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NEWS	2	JAN 02	STN pricing information for 2008 now available
NEWS	3	JAN 16	CAS patent coverage enhanced to include exemplified prophetic substances
NEWS	4	JAN 28	USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats
NEWS	5	JAN 28	MARPAT searching enhanced
NEWS	6	JAN 28	USGENE now provides USPTO sequence data within 3 days of publication
NEWS	7	JAN 28	TOXCENTER enhanced with reloaded MEDLINE segment
NEWS	8	JAN 28	MEDLINE and LMEDLINE reloaded with enhancements
NEWS	9	FEB 08	STN Express, Version 8.3, now available
NEWS	10	FEB 20	PCI now available as a replacement to DPCI
NEWS	11	FEB 25	IFIREF reloaded with enhancements
NEWS	12	FEB 25	IMSPRODUCT reloaded with enhancements
NEWS	13	FEB 29	WPINDEX/WPIDS/WPIX enhanced with ECLA and current U.S. National Patent Classification
NEWS	14	MAR 31	IFICDB, IFIPAT, and IFIUIDB enhanced with new custom IPC display formats
NEWS	15	MAR 31	CAS REGISTRY enhanced with additional experimental spectra
NEWS	16	MAR 31	CA/CAPLUS and CASREACT patent number format for U.S. applications updated
NEWS	17	MAR 31	LPCI now available as a replacement to LDPCI
NEWS	18	MAR 31	EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS	19	APR 04	STN AnaVist, Version 1, to be discontinued
NEWS	20	APR 15	WPIDS, WPINDEX, and WPIX enhanced with new predefined hit display formats
NEWS EXPRESS	FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3, AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008		
NEWS HOURS	STN Operating Hours Plus Help Desk Availability		
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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 17:16:33 ON 24 APR 2008

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FILE 'REGISTRY' ENTERED AT 17:20:02 ON 24 APR 2008

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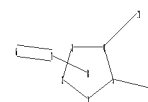
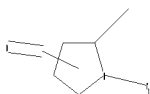
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6 7 9
ring nodes :
1 2 3 4 5
ring/chain nodes :
11
chain bonds :
4-11 5-9 6-7
ring bonds :
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exact bonds :
4-11

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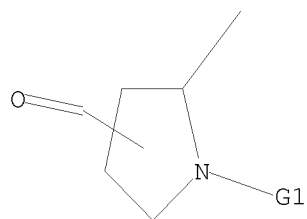
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L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR



G1 Cy,Hy

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss full

FULL SEARCH INITIATED 17:30:48 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 2432103 TO ITERATE

39.1% PROCESSED 950317 ITERATIONS 499 ANSWERS

41.1% PROCESSED 1000000 ITERATIONS 535 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.28

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**

PROJECTED ITERATIONS: 2432103 TO 2432103

PROJECTED ANSWERS: 1193 TO 1409

L2 535 SEA SSS FUL L1

=> file capl

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=> s 12

L3 73 L2

=> d 13 53-73 ibib abs hitstr

L3 ANSWER 53 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:582909 CAPLUS

DOCUMENT NUMBER: 141:218310

TITLE: Insights into Phenylalanine Derivatives Recognition of VLA-4 Integrin: From a Pharmacophoric Study to 3D-QSAR and Molecular Docking Analyses

AUTHOR(S): Macchiarulo, Antonio; Costantino, Gabriele; Meniconi, Mirco; Pleban, Karin; Ecker, Gerhard; Bellocchi, Daniele; Pellicciari, Roberto

CORPORATE SOURCE: Dipartimento di Chimica e Tecnologia del Farmaco, Universita di Perugia, Perugia, 06127, Italy

SOURCE: Journal of Chemical Information and Computer Sciences (2004), 44(5), 1829-1839
CODEN: JCISD8; ISSN: 0095-2338

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The very late antigen-4 (VLA-4), also known as integrin $\alpha 4\beta 1$, is expressed on monocytes, T- and B-lymphocytes, basophils, and eosinophils and is involved in the massive recruitment of granulocytes in different pathol. conditions such as multiple sclerosis and asthma. VLA-4 interacts with its endogenous ligand VCAM-1 during chronic inflammation, and blockade of VLA-4 /VCAM-1 interaction is a potential target for immunosuppression. Two classes of VLA-4 antagonists have so far been reported: β -amino acid derivs. containing a diaryl urea moiety (BIO-1211) and phenylalanine derivs. (TR-14035). With the aim of clarifying the structural basis responsible for VLA-4 recognition by phenylalanine derivs., the authors developed a combined computational study on a set of 128 antagonists available through the literature. Our computational approach is composed of three parts. (i) A VCAM-1 based pharmacophore was constructed with a restricted number of phenylalanine derivs. to identify the region of the protein that resembles synthetic antagonists. The pharmacophore was instrumental in constructing an alignment of a set of 128 compds. This alignment was exploited to build a pseudoreceptor model with the RECEPTOR program. (ii) 3D-QSAR anal. was carried out on the computed electrostatic and steric interaction energies with the pseudoreceptor surface. The 3D-QSAR anal. yielded a predictive model able to explain much of the variance of the 128 antagonists. (iii) A homol. modeling study of the headpiece of VLA-4 based on the crystal structure of $\alpha v\beta 3$ was performed. Docking expts. of TR-14035 into the binding site of VLA-4 aided the interpretation of the 3D-QSAR model. The obtained results will be fruitful for the design of new potent and selective antagonists of VLA-4.

IT 737804-72-7

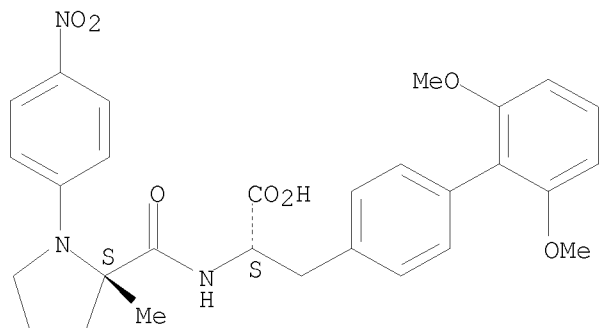
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(3D-QSAR and mol. docking analyses of phenylalanine derivs. recognition of VLA-4 integrin)

RN 737804-72-7 CAPLUS

CN L-Alanine, 2-methyl-1-(4-nitrophenyl)-L-prolyl-3-(2',6'-dimethoxy[1,1'-biphenyl]-4-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 54 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1966:59736 CAPLUS

DOCUMENT NUMBER: 64:59736

ORIGINAL REFERENCE NO.: 64:11149g-h,11150a-e

TITLE: 1,3-Cycloadditions of azomethinyllides from aziridinecarboxylic esters

AUTHOR(S): Huisgen, Rolf; Scheer, Wolfgang; Szeimies, Guenter; Huber, Helmut

CORPORATE SOURCE: Univ. Munich, Germany

SOURCE: Tetrahedron Letters (1966), (4), 397-404

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: German

GI For diagram(s), see printed CA Issue.

AB cf. Heine and Peavy, CA 63, 14796e. By a ring opening between the 2 and 3 positions, di-Me 1-(p-methoxyphenyl)aziridine-2,3-dicarboxylate (I) adds to C:C and C.tplbond.C compds. to give pyrrolidine or pyrroline derivs. Heating di-Me 1-(p-methoxyphenyl)-Δ²-1,2,3-triazoline-4,5-trans-dicarboxylate at 100° gives I as a 15:85 cis-trans mixture. The reactions and epimerizations of I presumably proceed through the intermediate formation of epimers of MeO₂CCH: N+(p-MeOC₆H₄)C-HCO₂Me. Heating di-Me fumarate (II) and I at 140° yields 94% tetra-Me 1(p-methoxyphenyl)pyrrolidine-2,3,4,5-tetracarboxylate (III) containing an oily isomer (IIIa) and 59% of a crystalline isomer (IIIb), m. 112-13°. IIIa and IIIb are dehydrogenated by chloranil (IV) in boiling Decalin to give 21 and 22% yields, resp., of tetra-Me 1-(p-methoxyphenyl)pyrrole-2,3,4,5-tetracarboxylate, independently synthesized by the method of Huntress, et al. (CA 50, 12977b) from p-MeOC₆H₄NHOH and (MeO₂CC.tplbond.)₂. III is also prepared in 61% yield from II and p-MeOC₆H₄N₃ at 100-140°. At 120°, I and [(EtO₂C)₂CH:]₂ give 77% of 2,5-di-Me 3,3,4,4-tetra-Et 1-(p-methoxyphenyl)pyrrolidine-2,3,3,4,4,5-hexacarboxylate containing 65% of the cis form, m. 114-15°, and 35% of the trans form, m. 114-16°, separated on silica gel by 9:1 C₆H₆-Et₂O. The addition of norbornene to I at 100° gives 94% V containing 63% cis form (V, R = CO₂Me, R₁ = H), an oil, and 37% trans form (V, R = H, R₁ = CO₂Me), m. 87-9°, separated by thin layer chromatography. IV in boiling cymene converts V to VI, m. 161-2°. At 125°, I combines with HC.tplbond.CH in Me₂CO to give an 81% yield of adducts, presumably a mixture of Δ²- and Δ³-pyrrolines which are dehydrogenated by IV in boiling xylene to give a 68% yield of di-Me 1-(p-methoxyphenyl)pyrrole-2,5-dicarboxylate, identical to the product obtained from p-MeOC₆H₄NH₂ and di-Me α,α'-dihydroxy muconate (Kuhn and Dury, CA 45, 7017a). BzC.tplbond.CPh and I at 100° yield 93% of an adduct dehydrogenated by IV in PhMe to give 55% di-Me ester of 3-benzoyl-1-(p-methoxyphenyl)-4-

phenylpyrrole-2,5-dicarboxylic acid (VII). VII decarboxylates at 200° to give 3-benzoyl-1-(4-methoxyphenyl)-4-phenylpyrrole (VIII), characterized by its 2,4-dinitrophenylhydrazone. VIII is also prepared by condensing the Na derivative of BzCH₂CHO with p-MeOC₆H₄NHCH₂Bz, and cyclizing the product with concentrated H₂SO₄. Photochem. or thermally (150°), I dimerizes to give a mixture from which two isomers, m. 188-9° and 240-1°, of tetra-Me 1,4-bis(p-methoxyphenyl)piperazine-2,3,5,6-tetracarboxylate have been isolated. Heating Me 1-phenylaziridine-2-carboxylate (IX) 6 hrs. at 200° gave 50% of the di-Me ester of 1,4-diphenylpiperazine-2,3-trans-dicarboxylic acid (X), m. 132-3°, and 5% of the cis ester, m. 105-6°. Distillation of Ca salt of X yields (PhNHCH₂)₂ and 1,4-diphenylpiperazine. The reaction of IX with trans-(BzCH₂)₂ (XI) gives a 1:1 adduct, m. 120-1°, and with PhCH:NMe, an adduct, m. 132.5-4° (structures not given). The addition of 1-benzyl-2,3-trans-dibenzoylaziridine to XI gives 34% of 1-benzyl-2,3,4,5-(all-trans)-tetrabenzoylpyrrolidine.

IT 875613-01-7P, 4,7-Methanoisindoline-1,3-dicarboxylic acid, hexahydro-2-(p-methoxyphenyl)-, dimethyl ester, cis-

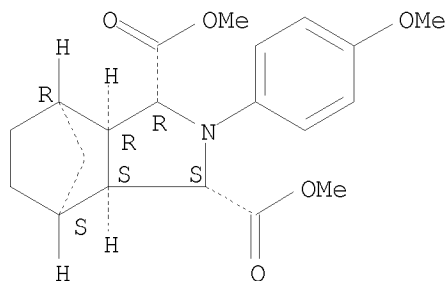
RL: PREP (Preparation)

(preparation of)

RN 875613-01-7 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

Relative stereochemistry.



L3 ANSWER 55 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1956:64500 CAPLUS

DOCUMENT NUMBER: 50:64500

ORIGINAL REFERENCE NO.: 50:12020g-i

TITLE: Synthesis of spasmolytic substances. X. Synthesis of some alkylamino esters of pyrrolidine-2,5-dicarboxylic acid

AUTHOR(S): Klosa, Josef

SOURCE: Arch. Pharm. (1955), 288, 72-4

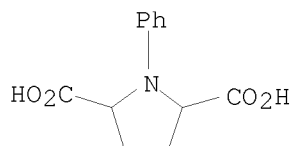
DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. C.A. 49, 8274d. Adipic acid (100 g.) and 200 cc. SOCl₂ heated 2 hrs. on the steam bath, the volatile products removed in vacuo, the residual oily product brominated at 50° under ultraviolet light with 200 g. of Br and the product allowed to stand 24 hrs. with 700 cc. absolute EtOH gave 90 g. di-Et 2,5-dibromoadipate (I), m. 65-7° (from benzene). Di-Me 2,5-dibromoadipate, prepared similarly, m. 75-7°. I (10 g.) and 30 g. aniline refluxed 18 hrs. in 100 cc. benzene, and fractionally distilled gave 7 g. di-Et 1-phenyl-2,5-pyrrolidinedicarboxylate (II), b₂ 230-40°. The di-Me ester, b₂ 250-60°, m. 85-7°, and di-Et 1-butyl-2,5-pyrrolidinedicarboxylate, b₂ 156-8°, were prepared similarly. II (20 g.) refluxed 24 hrs. with 100 g. Et₂NCH₂CH₂OH, and the mixture fractionally distilled gave 12 g. of 1-phenyl-2,5-pyrrolidinedicarboxylic acid di(β-diethylaminoethyl) ester, b₁

193-5°. The following di(β -diethylaminoethyl) esters of 2,5-pyrrolidinedicarboxylic acid were prepared similarly: 1-butyl, 60%, b1 168-9°; 1-methyl, 43%, b1 174-7°; 1-benzyl, 52%, b1 200-3°; and 1-propyl, 35%, b1 167-70°.

IT 859957-82-7, 2,5-Pyrrolidinedicarboxylic acid, 1-phenyl-
(esters)
RN 859957-82-7 CAPLUS
CN 2,5-Pyrrolidinedicarboxylic acid, 1-phenyl- (CA INDEX NAME)



L3 ANSWER 56 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1956:20042 CAPLUS
DOCUMENT NUMBER: 50:20042
ORIGINAL REFERENCE NO.: 50:4125d-i, 4126a-b
TITLE: 2,3-Pyrrolidinediones. IV. Further studies on tautomerism
AUTHOR(S): Vaughan, Wyman R.; McCane, Donald I.
CORPORATE SOURCE: Univ. of Michigan, Ann Arbor
SOURCE: Journal of Organic Chemistry (1955), 20, 143-54
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 50:20042

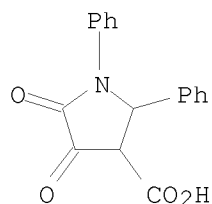
AB cf. C.A. 48, 3340i. Addnl. evidence has been presented that 1,5-diaryl-2,3-pyrrolidinediones are tautomeric with α -arylimino- β -arylidene propionic acids and that it is the latter which undergo thermal decarboxylation. Refluxing 14.4 g. 1,4-diphenylazetidinone overnight in 125 cc. MeOH saturated with HCl, evaporating the mixture in vacuo, and treating the residue with H₂O and a little NaHCO₃ give 86.5% Me β -phenyl- β -phenylaminopropionate, needles, m. 105-6°, which (5.1 g.) is treated in 50 cc. dry (CH₂Cl)₂ containing 15 cc. C₅H₅N 3 hrs. at 20° with 3 cc. MeO₂CCOCl, the mixture is diluted with 50 cc. Et₂O, and the residue of the washed (H₂O, 5% HCl-H₂O) and dried Et₂O solution evaporated, giving 95% Me β -phenyl- β -(N-methoxalyl-N-phenylamino)-propionate (I), m. 75.5-6°. Adding MeONa (from 0.07 g. Na) in 20 cc. absolute MeOH to 0.9 g. I, keeping the mixture 4 hrs., neutralizing it with the calculated amount of AcOH in 50 cc. H₂O, and extracting with Et₂O give 0.5 g. 4-carbomethoxy-1,5-diphenyl-2,3-pyrrolidinedione (II), m. 196-9° (decomposition); it gives a deep red color with FeCl₃. Adding 2 g. Me methoxalylacetate to 50 cc. Et₂O containing 2 g. PhCH:NPh and evaporating the filtered solution give II. Refluxing a sample of the Et ester of II in PhNO₂ gives 1 mole CO₂ and 1,5-diphenyl-2,3-pyrrolidinedione (III). Heating 22.5 g. CuCl₄N with 37 g. AcBr 2 hrs. at 70-80° gives 54.3% MeCOC₁₄N, b. 87-91°, which (9 g.) is treated at 0° with 12.5 cc. concentrated HCl, and the mixture diluted with 40 cc. H₂O and heated 2 hrs. at 70°, giving 38% MeCOC₁₄O₂H (IV), b18 40-60°. Adding 1 g. IV to 5 cc. 10% NaOH, then adding at 0° 1.2 g. BzH and, dropwise (10 min.), 3 cc. 10% NaOH, and stirring the mixture 50 min. with the temperature kept below 12° give 0.9 g. PhCH:CHCOC₁₄O₂Na which, dissolved in 20 cc. ice H₂O, is decomposed with 25 drops concentrated HCl in 10 cc. ice-H₂O, giving

47% PhCH: CHCOC14O2H (V), m. 68-9°. Adding 0.36 g. PhNH2 in 5 cc. absolute EtOH dropwise to 0.67 g. V in 15 cc. absolute EtOH, stirring the mixture 0.5 hr. at 20°, diluting it with 25 cc. EtOH, and refluxing it 1 hr. give 80% III-2-C14 (VI), m. 158-60° (decomposition). o-C6H4(CO)2N15H is converted into PhN15H2 which, with PhCH:CHCOCO2H, gives III-1-N15 (VII). Refluxing 2.51 g. VII in 25 cc. absolute EtOH 0.5 hr. with 1.1 g. PhNHNH2 in 10 cc. absolute EtOH and 4 drops AcOH, keeping the mixture 12 hrs. at 20%, refluxing it another hr., and diluting the cooled solution with 70 cc. H2O give 79% inactive 1-anilino-5-phenyl-2,3-pyrrolidinedione (VIII), m. 154-5° (decomposition); the mother liquor is extracted with C6H6 and HCl is passed into the extract, giving PhN15H2.HCl (IX). Treating III with PhNHN15H2 (X) (prepared from PhNH2 and KN15O3) gives 75% active VIII, m. 154.5-6° (decomposition). For the collecting of N for mass spectrometric analysis 0.39 g. PhNH2.HCl, 6 g. 50% H3PO2, and 10 cc. H2O are treated at 5° with 0.21 g. NaNO2 in 10 cc. H2O. The decarboxylation of VI is carried out by heating 0.251 g. in 20 cc. o-C6H4Cl2 1 hr. at 180° (bath temperature), absorbing the CO2 in 1N NaOH by means of a CO2-free N stream, and precipitating it as BaCO3. This gives BaC14O3 with 94.9% of the starting C14, indicating that VI is thermally decarboxylated to cinnamylideneaniline and C14O2 by initial rearrangement to the isomeric 3-arylidene-2-aryliminopropionic acids. In the reaction of III with X active VIII is formed by an exchange between tautomeric arylimino acid and X.

IT 873399-08-7, 3-Pyrrolidinecarboxylic acid, 4,5-dioxo-1,2-diphenyl- (esters)

RN 873399-08-7 CAPLUS

CN 3-Pyrrolidinecarboxylic acid, 4,5-dioxo-1,2-diphenyl- (CA INDEX NAME)



L3 ANSWER 57 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1955:46203 CAPLUS

DOCUMENT NUMBER: 49:46203

ORIGINAL REFERENCE NO.: 49:8908f-i,8909a-b

TITLE: Pyrrolidine esters

AUTHOR(S): Van Heyningen, Earle M.

CORPORATE SOURCE: Eli Lilly & Co., Indianapolis, IN

SOURCE: Journal of the American Chemical Society (1954), 76, 3043-4

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

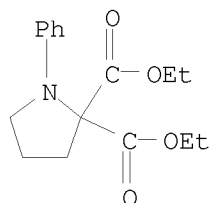
LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 49:46203

AB The condensation of 1,3-dibromoalkanes with an aminomalonate in refluxing EtOH with NaOEt yielded the corresponding 2,2-dialkoxypyrrolidines in fair yields. The yields could be improved considerably by effecting the cyclization in a nonhydroxylic solvent using NaNH2. Na (14.1 g.) dissolved in 350 cc. absolute EtOH, the solution treated with 107 g. H2NCH(CO2Et)2 and then with 246.5 g. Br(CH2)3Br in large portions, the mixture refluxed 4 hrs., the EtOH removed in vacuo, the residue dissolved in dilute HCl, the acid solution extracted with Et2O to recover the unreacted Br(CH2)3Br (90 g.), basified with dilute aqueous NaOH, and extracted with Et2O, and

the extract dried and distilled yielded 28.8 g. (22%) 2,2-dicarbethoxypyrrolidine (II), b₂ 105°, n_{25D} 1.4455. II in Et₂O treated with dry HCl gave II.HCl, white needles, m. 91-2° (from Et₂O-CHCl₃). I (135.5 g.) and then 357 g. (MeCHBr)₂CH₂ (III) added to 18 g. Na in 450 cc. absolute EtOH, and the mixture refluxed 12 hrs. and worked up in the usual manner gave 250 g. recovered III and 66.3 g. (35.6%) 3,5-di-Me derivative (IV) of II, b₁ 91-4°, n_{25D} 1.4447. NaNH₂ prepared from 36 g. Na in 1 l. liquid NH₃, the NH₃ evaporated and replaced by 500 cc. dry C₆H₆ which was refluxed to remove traces of NH₃, the mixture treated with 136.7 g. I, gently warmed to remove all of the NH₃ while being bubbled with dry N, treated dropwise with stirring with 200 g. III, refluxed 26 hrs., cooled, diluted with H₂O, and extracted with C₆H₆, and the extract washed and distilled yielded 128.2 g. (67.7%) IV, b_{0.76} 89-93°, n_{25D} 1.4455. IV in dry Et₂O treated with dry HCl gave IV.HCl, m. 105-7° (from CHCl₃-Et₂O). IV (66.3 g.) added to a suspension of NaNH₂ (from 6.45 g. Na in liquid NH₃) in 200 cc. PhMe, and the mixture heated 15 hrs. and worked up in the usual manner gave 29.8 g. (42.5%) IV, b_{0.8-1.1} 99-105°, n_{25D} 1.4515. NaNH₂ (from 4.6 g. Na) suspended in 200 cc. PhMe and treated with 25.3 g. PhNHCH(CO₂Et)₂, the NH₃ removed, the residual mixture treated with 20.1 g. Br(CH₂)₃Br and refluxed gave similarly 8.0 g. (27.5%) 1-Ph derivative of II, b_{0.6} 145°, n_{25D} 1.5132. NaNH₂ (from 27.6 g. Na) suspended in 700 cc. PhMe treated with 100 g. NC(AcNH)CHCO₂Et, the NH₃ removed, and the mixture treated with 121.5 g. Br(CH₂)₃Br and worked up in the usual manner yielded 54.0 g. (43.5%) 1-acetyl-2-carbethoxy-2-cyanopyrrolidine (V), b₁ 163°, n_{25D} 1.4765. V (15 g.) refluxed 8 hrs. with 9.65 g. guanidine carbonate in EtOH containing NaOEt, and the liquid mixture decanted into H₂O gave 9 g. spiro[1-acetylpyrrolidine-2,5'-(2,4-diiminobarbituric acid)], m. 311-12° (from H₂O).

IT 860360-20-9P, 2,2-Pyrrolidinedicarboxylic acid, 1-phenyl-, diethyl ester
 RL: PREP (Preparation)
 (preparation of)
 RN 860360-20-9 CAPLUS
 CN 2,2-Pyrrolidinedicarboxylic acid, 1-phenyl-, 2,2-diethyl ester (CA INDEX NAME)



L3 ANSWER 58 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1954:60443 CAPLUS
 DOCUMENT NUMBER: 48:60443
 ORIGINAL REFERENCE NO.: 48:10733g-i,10734a-i,10735a-b
 TITLE: The condensation of oxalic esters with esters of β-alanine and N-substituted 3-aminopropionic acids. Synthesis of some derivatives of 2,3-dioxopyrrolidine and 2-oxo-3-methoxy-3-pyrroline
 AUTHOR(S): Southwick, Philip L.; Crouch, Robert T.
 CORPORATE SOURCE: Carnegie Inst. of Technol., Pittsburgh, PA
 SOURCE: Journal of the American Chemical Society (1953), 75, 3413-17
 CODEN: JACSAT; ISSN: 0002-7863
 DOCUMENT TYPE: Journal

LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 48:60443

AB The condensation of (CO₂Me)₂ or (CO₂Et)₂ with a series of N-substituted 3-aminopropionic acid esters yielded a series of 1-substituted 4-carbomethoxy- and 4-carbethoxy-2,3-dioxopyrrolidines (I), converted into 4-carbalkoxy-2-oxo-3-methoxy-3-pyrrolines by treatment with CH₂N₂. The 4-carbalkoxy-1-benzyl-2,3-dioxopyrrolidines were hydrolyzed and decarboxylated to 1-benzyl-2,3-dioxopyrrolidine (II). Cyclohexylamine (49.5 g.) and 43 g. freshly distilled CH₂:CHCO₂Me (III) in 400 cc. absolute

MeOH

let stand 24 hrs., the solvent distilled off, and the residual oil fractionated gave 83 g. (90%) Me 3-(cyclohexylamino)propionate, b₄₋₅ 125-8°, giving in dry C₆H₆ with dry HCl the HCl salt, white needles, m. 163-4° (from MeOH). Similarly was prepared the corresponding Et ester (IV), b₃₋₅ 133-5°, 85%; [HCl salt, colorless needles, m. 145-6° (from absolute EtOH)], and Me 3-(benzylamino)propionate (V), b₇ 145-7° 92%; [HCl salt, white plates, m. 164-5° (from MeOH)]. p-MeC₆H₄NH₂ (35.3 g.), 28.4 g. III, 40 cc. dry C₆H₆, and 10 drops SnCl₄ refluxed 24 hrs. yielded 42.5 g. (67%) p-MeC₆H₄NH(CH₂)₂CO₂Me, b₅₋₆ 145-50°, m. 60-1°, light yellow plates from C₆H₆-petr. ether. p-MeC₆H₄NH₂ (53.5 g.), 50 g. freshly distilled CH₂:CHCO₂Et, and 20 g. glacial AcOH refluxed 24 hrs., and the resulting deep red solution distilled gave 52 g. (50%) p-MeC₆H₄NH(CH₂)₂CO₂Et, b₂₋₃ 142-4°; HCl salt, white needles, m. 92-3° (from absolute EtOH). Similarly was prepared PhNH(CH₂)₂CO₂Et, 63%, b₁₋₂ 139-46°; HCl salt, m. 98-9°. To 5.4 g. NaOMe in 50 cc. dry Et₂O was added with stirring 11.8 g. (CO₂Me)₂ and then 19.3 g. V in 50 cc. Et₂O, the mixture refluxed 0.5 hr. with stirring, the Et₂O distilled off, the residual salt taken up in 500 cc. warm H₂O, the mixture acidified with dilute HCl, let stand several hrs., filtered, and the residue recrystd. from MeOH to yield 18 g. (75%) 4-carbomethoxy-1-benzyl-2,3-dioxopyrrolidine (VI), white needles, m. 180-2° [recrystd., m. 183-4° (from MeOH)]. Similarly were prepared the following 1-substituted-4-carbomethoxy-2,3-dioxopyrrolidines (1-substituent, % yield, and m.p. given): p-MeC₆H₄, colorless needles, 45, 193-4° (from MeOH); m-ClC₆H₄, colorless needles, 29, 185-6° (from MeOH); p-MeOC₆H₄, yellow needles, 30, 209-10° (from MeOH); cyclohexyl, colorless needles, 29, 178-9° (from MeOH); and 1-phenyl-4-carbethoxy-2,3-dioxopyrrolidine, colorless needles, 48, 153° (from EtOH). Et 3-(cyclohexylamino)propionate (19.9 g.) and 14.6 g. (CO₂Et)₂ refluxed 1 hr. on the steam bath with 6.8 g. NaOEt, the resulting solid filtered off, washed with Et₂O, suspended in 500 cc. warm H₂O, acidified, let stand several hrs., filtered, and the filter residue recrystd. from 95% EtOH yielded 16.5 g. (65%) 1-cyclohexyl-4-carbethoxy-2,3-dioxopyrrolidine, white needles, m. 185-6° (recrystd., m. 188°). Similarly were prepared the following 1-substituted-4-carbethoxy-2,3-dioxopyrrolidines (1-substituent, % yield, and m.p. given): p-MeC₆H₄ (VII), colorless needles, 52, 156° (from EtOH); m-ClC₆H₄, colorless needles, 37, 142-3° (from EtOH); p-MeOC₆H₄, yellow needles, 55, 160-1° (from EtOH); and PhCH₂, (VIII), colorless needles, 75, 135-6° (from EtOH). PhNH(Ph)CHCH₂CO₂Et (10.3 g.) and 6.1 g. (CO₂Et)₂ in 25 cc. absolute EtOH added to 2.8 g. NaOEt in 50 cc. absolute EtOH, the EtOH distilled off on

the

steam bath, the light tan liquid residue dissolved in 300 cc. warm H₂O, the solution acidified with 20% HCl, and the light tan solid precipitate recrystd.

from EtOH gave 9 g. (73%) 4-carbethoxy-1,5-diphenyl-2,3-dioxopyrrolidine, white needles, m. 172-4°. Similarly was prepared 4-carbethoxy-2,3-dioxopyrrolidine, white plates, 72%, m. 185-6° (from EtOH) preheated to 175°. VII (2 g.) in 10 cc. Et₂O treated with excess CH₂N₂ in Et₂O, the excess CH₂N₂ destroyed with AcOH, the Et₂O evaporated, and the residual light yellow oil recrystd. from EtOH gave 2 g.

(95%) 4-carbomethoxy-1-p-tolyl-3-methoxy-2-oxo-3-pyrroline, colorless needles, m. 82-3° (from EtOH). Similarly were prepared the following 1-substituted-4-carbomethoxy-2-oxo-3-methoxy-3-pyrrolines (1-substituent, % yield, and m.p. given): m-ClC₆H₄, colorless needles, 91, 140-1° (from EtOH); p-MeOC₆H₄, colorless needles, 95, 109-10° (from EtOH); cyclohexyl, colorless needles, 91, 86-7° (from EtOH); Ph, colorless needles, 95, 76-7° (from EtOH); H, colorless needles, 74, 105-6° (from MeOH); and the following 1-substituted-4-carbomethoxy-2-oxo-3-methoxy-3-pyrrolines: p-MeC₆H₄, colorless needles, 95, 141-2° (from MeOH); m-ClC₆H₄, colorless needles, 86, 115-16° (from MeOH); p-MeOC₆H₄, light yellow needles, 94, 133-4° (from MeOH); cyclohexyl, colorless needles, 95, 103-4° (from MeOH); PhCH₂, colorless needles, 95, 77-8° (from MeOH). Ph(MeO₂CCO)NCH(Ph)CH₂CO₂Me (5 g.) in 50 cc. dry MeOH treated with 0.81 g. NaOMe in 25 cc. MeOH, and the precipitated white gelatinous Na salt filtered

off

and triturated with AcOH gave 1 g. PhNHCOCO₂Me, m. 111-12°; the filtrate from the Na salt evaporated to dryness, the residual solid extracted

with

H₂O, the aqueous extract acidified, and the resulting precipitate recrystd.

from MeOH

gave 0.4 g. (9%) 4-carbomethoxy-1,5-diphenyl-2,3-dioxopyrrolidine, m. 199-200°; the residue (0.3 g.) from the H₂O extraction was PhCH:CHCO₂Me, m. 32-3°. VIII (2 g.) and 150 cc. 20% HCl refluxed 3 hrs., the mixture cooled, filtered, extracted several times with CHCl₃, the CHCl₃

evaporated,

and the light tan oily residue crystallized from C₆H₆ gave 1.2 g. (83%) 1-benzyl-2,3-dioxopyrrolidine, white needles, m. 99-100°, also obtained in 69% yield from VI by a similar hydrolysis. PhCH₂NH(CH₂)₂CO₂Et (30 g.) and 150 cc. 10% NaOH refluxed until the ester layer disappeared, the solution neutralized with dilute HCl, evaporated to dryness, the white

solid

residue extracted with boiling absolute EtOH, and the extract cooled gave 22.5

g.

(87%) PhCH₂NH(CH₂)₂CO₂H (IX), white needles, m. 182-3°. IX (5 g.) and 10 g. MeO₂CCOCl heated 0.5 hr. on the steam bath, the solution diluted with 100 cc. Et₂O, washed with H₂O, extracted with excess 5% aqueous NaHCO₃, the

alkaline

extract acidified, the precipitated light yellow oil let stand, and the

resulting

solid recrystd. from CHCl₃-petr. ether yielded 5 g. (68%)

Ph-CH₂N(COCO₂Me)CH₂CH₂CO₂H (X), white plates, m. 99-100°. X (8 g.)

and 8 g. MeO₂CCOCl in 25 cc. anhydrous CHCl₃ treated with 8 g. pyridine, the solution let stand 2 hrs., washed with H₂O, heated on the steam bath with 400 cc. 5% aqueous NaHCO₃, the aqueous extract decolorized with C, filtered, the

filtrate

acidified, an unidentified precipitated acid (XI) (2.2 g.) filtered off, the filtrate extracted with CHCl₃, and the extracted evaporated gave 0.5 g.

1-benzyl-2-oxo-3-methoxy-3-pyrroline-4-carboxylic acid, m. 139-40°

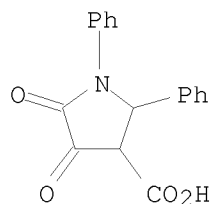
(from CHCl₃-petr. ether), esterified with CH₂N₂ to VI, m. 77-8°.

XI dissolved in aqueous KOH, repptd. with HCl, and recrystd. from aqueous EtOH gave small pale yellow plates, m. 245-6°.

IT 873399-08-7, 3-Pyrrolidinecarboxylic acid, 4,5-dioxo-1,2-diphenyl-
(esters)

RN 873399-08-7 CAPLUS

CN 3-Pyrrolidinecarboxylic acid, 4,5-dioxo-1,2-diphenyl- (CA INDEX NAME)



L3 ANSWER 59 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1953:25510 CAPLUS

DOCUMENT NUMBER: 47:25510

ORIGINAL REFERENCE NO.: 47:4373g-i, 4374a-e

TITLE: Amino esters of 1-substituted 2,5-pyrrolidinedicarboxylic acids

INVENTOR(S): Hill, Arthur J., Jr.; Maynard, John T.

PATENT ASSIGNEE(S): American Cyanamid Co.

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2596099		19520513	US 1946-719108	19461228

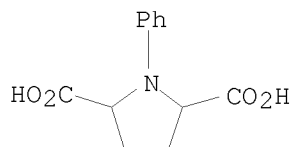
AB Dialkyl dibromoadipates with primary amines give esters of 1-substituted 2,5-pyrrolidinedicarboxylic acids, and the products undergo ester interchanges with tertiary amino alcs. according to the following processes. PhNH₂ 3.5 refluxed with meso-(MeO₂CCHBrCH₂)₂ 1 mole gives 68% di-Me 1-phenyl-2,5-pyrrolidinedicarboxylate, b₂₇ 220-30°, m. 88°. A solution of BuNH₂ 3 and meso-(EtO₂CCHBrCH₂)₂ (I) 1 mole in C₆H₆ allowed to heat spontaneously, refluxed to complete the reaction, treated with a little Et₂O, freed of salt, extracted with 6 N H₂SO₄, the extract neutralized with Na₂CO₃, and the oil taken up in Et₂O and distilled give 60% 1-butyl-2,5-dicarbethoxypyrrolidine, b₁₋₂ 155-6°, n_{D20} 1.4514. PhNH₂ 327, I 360, and KI 5 parts are warmed gently to initiate a violent reaction, then heated at 85-90°, the product suspended in 6 N HCl, extracted with Et₂O, and the exts. washed, dried, filtered, and distilled to give 90% di-Et 1-phenyl-2,5-pyrrolidinedicarboxylate, b_{0.5} 144°, n_{D21.5} 1.5230. 1 30, cyclohexylamine (II) 25, pulverized KI 1, and C₆H₆ 75 parts let stand several hrs., refluxed, cooled, the mixture filtered, extracted with 70 cc. of 6 N H₂SO₄, the extract neutralized with Na₂CO₃, and the oil taken up in Et₂O and distilled give 85.5% 1-cyclohexyl-2,5-dicarbethoxypyrrolidine (III), b₁ 133°, n_{D20} 1.4738. 0 Similarly, I 1, II 1, pulverized K₂CO₃ 1 mole, and a little KI in 9 hrs. give 50% III; extending the reaction time to 52 hrs. gives 54% III. Other 1-substituted-2,5-dicarbethoxypyrrolidines prepared are: Me, b₂₃ 158-63°, n_{D20} 1.4595; Et, b₃₋₄ 119-21°, n_{D20} 1.4530; Pr, b₅ 130-1°, n_{D20} 1.4503; iso-Bu, b_{1-1.5} 115-16°, n_{D20} 1.4498; hexyl, b₁ 117°, n_{D20} 1.4529; benzyl, b₁ 138°, n_{D20} 1.5042; 2-methoxyethyl, b₁ 108-9°, n_{D20} 1.4550; phenethyl, b₁ 154-5°, n_{D20} 1.5026; 2-acetamidoethyl, b₁ 168°, n_{D20} 1.4657; Ph(alkyl-methyl)(?), m. 88°; o-tolyl, b_{0.5} 129-30°, n_{D20} 1.5108; m-tolyl, b_{0.5} 136-7°, n_{D21.5} 1.5215; p-tolyl, b_{0.5} 164-5°, n_{D21.5} 1.5226; p-ClC₆H₄ b_{0.5} 158°, n_{D21.5} 1.5342; 2,4-Me₂C₆H₃, b_{0.5} 135-6°, n_{D21.5} 1.5081; 3,5-Me₂C₆H₃, b_{0.5} 145-6°, n_{D21.5} 1.5170; p-Ac-NHC₆H₅, decomposition 136°, n_{D21.5} 1.5417; p-AcC₆H₄, decompose 136°, n_{D21.5} 1.5459. Na 1 in Et₂NCH₂CH₂OH (IV) 250 and the product

heated at 160-70° with 1-methyl-2,5-dicarbethoxypyrrolidine 53 parts gives 41% bis(2-diethyl-aminoethyl) 1-methyl-2,5-pyrrolidinedicarboxylate (V), b1 172-81°, nD20 1.4690. Similarly prepared are the 1-Et analog of V, b1 168.5-9° nD20 1.4678 (HCl salt, too hygroscopic to determine the m.p.); bis(3-diethylaminopropyl) 1-butyl-2,5-pyrrolidine-dicarboxylate (VI), b1 186°, nD20 1.4619; 60% of the 1-cyclohexyl analog of VI, b1 203-4°, nD20 1.4803; bis[2-(4-morpholinyl)ethyl] 1-butyl-2,5-pyrrolidinedicarboxylate; and the 1-benzyl analog of V, b0.5 196-8°, nD20 1.4985. Na 1.5 dissolved in IV 540 and the product heated at 165° with 1-phenyl-2,5-dicarbethoxypyrrolidine 100 parts gives the 1-Ph analog of V, b0.5 189-91°, nD21.5 1.5121. Similarly prepared are the following analogs of V: p-tolyl, b0.5 175-8°, nD21.5 1.5144; 2,4-Me2C6H3, b1 187-90°, nD21.5 1.5023; Pr, b0.2 154-5°, nD20 1.4660; Bu, b1 169-70°, nD20 1.4664; iso-Bu, b1 155-6°, nD20 1.4656; hexyl, b1 179-80°, nD20 1.4668; cyclohexyl, b1 198°, nD20 1.4820; MeOCH2CH2, b1 175-7°, nD20 1.4695; PhCH2CH2, b1 206°, nD20 1.5002; o-tolyl, b0.5 180°, nD21.5 1.5035; m-tolyl, b0.5 195-6°, nD21.5 1.5113; p-ClC6H4, b1 207-8°, nD21.5 1.5203; and 2,5-Me2C6H3, b0.5 198-200°, nD21.5 1.5092. The compds. prepared are useful as local anesthetics and antispasmodics.

IT 859957-82-7, 2,5-Pyrrolidinedicarboxylic acid, 1-phenyl-
 860360-08-3, 2,5-Pyrrolidinedicarboxylic acid, 1-cyclohexyl-
 860360-10-7, 2,5-Pyrrolidinedicarboxylic acid, 1-(p-chlorophenyl)-
 860360-52-7, 2,5-Pyrrolidinedicarboxylic acid, 1-(2,4-xyllyl)-
 860360-54-9, 2,5-Pyrrolidinedicarboxylic acid, 1-p-tolyl-
 860360-56-1, 2,5-Pyrrolidinedicarboxylic acid, 1-o-tolyl-
 860360-58-3, 2,5-Pyrrolidinedicarboxylic acid, 1-m-tolyl-
 (esters)

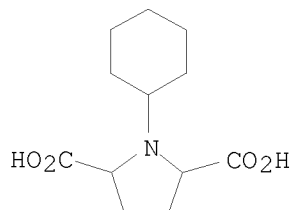
RN 859957-82-7 CAPLUS

CN 2,5-Pyrrolidinedicarboxylic acid, 1-phenyl- (CA INDEX NAME)



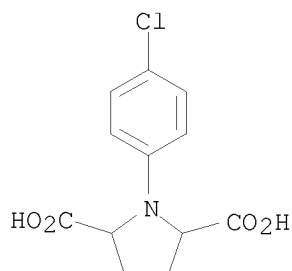
RN 860360-08-3 CAPLUS

CN 2,5-Pyrrolidinedicarboxylic acid, 1-cyclohexyl- (CA INDEX NAME)



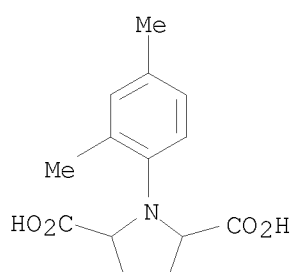
RN 860360-10-7 CAPLUS

CN 2,5-Pyrrolidinedicarboxylic acid, 1-(4-chlorophenyl)- (CA INDEX NAME)



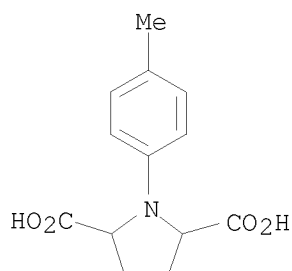
RN 860360-52-7 CAPLUS

CN 2,5-Pyrrolidinedicarboxylic acid, 1-(2,4-dimethylphenyl)- (CA INDEX NAME)



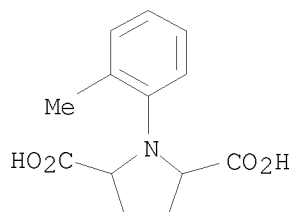
RN 860360-54-9 CAPLUS

CN 2,5-Pyrrolidinedicarboxylic acid, 1-(4-methylphenyl)- (CA INDEX NAME)



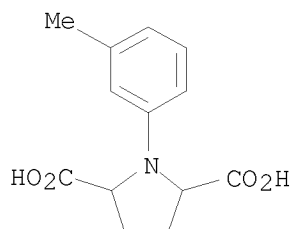
RN 860360-56-1 CAPLUS

CN 2,5-Pyrrolidinedicarboxylic acid, 1-(2-methylphenyl)- (CA INDEX NAME)

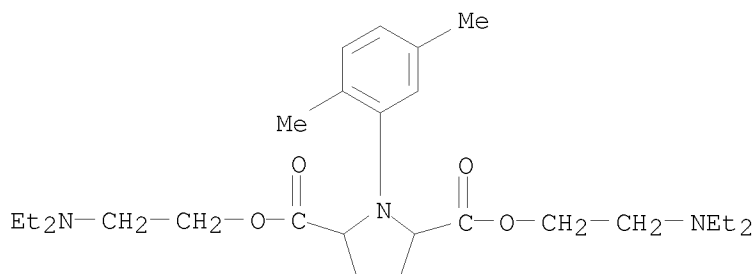


RN 860360-58-3 CAPLUS

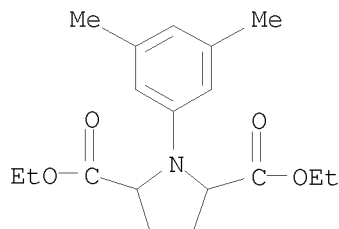
CN 2,5-Pyrrolidinedicarboxylic acid, 1-(3-methylphenyl)- (CA INDEX NAME)



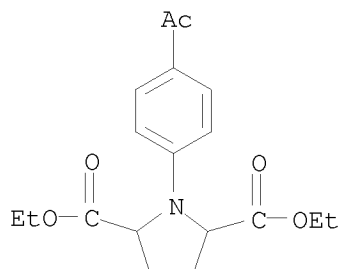
IT 857760-50-0P, 2,5-Pyrrolidinedicarboxylic acid, 1-(2,5-xylyl)-, bis(2-diethylaminoethyl) ester 857760-52-2P,
 2,5-Pyrrolidinedicarboxylic acid, 1-(3,5-xylyl)-, diethyl ester 860360-12-9P, 2,5-Pyrrolidinedicarboxylic acid, 1-(p-acetylphenyl)-, diethyl ester 860360-14-1P,
 2,5-Pyrrolidinedicarboxylic acid, 1-(p-acetamidophenyl)-, diethyl ester
 RL: PREP (Preparation)
 (preparation of)
 RN 857760-50-0 CAPLUS
 CN 2,5-Pyrrolidinedicarboxylic acid, 1-(2,5-dimethylphenyl)-, 2,5-bis[2-(diethylamino)ethyl] ester (CA INDEX NAME)



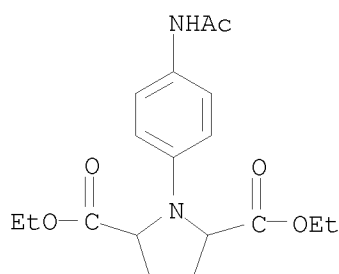
RN 857760-52-2 CAPLUS
 CN 2,5-Pyrrolidinedicarboxylic acid, 1-(3,5-dimethylphenyl)-, 2,5-diethyl ester (CA INDEX NAME)



RN 860360-12-9 CAPLUS
 CN 2,5-Pyrrolidinedicarboxylic acid, 1-(4-acetylphenyl)-, 2,5-diethyl ester (CA INDEX NAME)



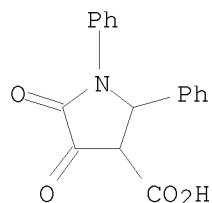
RN 860360-14-1 CAPLUS
 CN 2,5-Pyrrolidinedicarboxylic acid, 1-[4-(acetylamino)phenyl]-, 2,5-diethyl ester (CA INDEX NAME)



L3 ANSWER 60 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1949:46441 CAPLUS
 DOCUMENT NUMBER: 43:46441
 ORIGINAL REFERENCE NO.: 43:8380b-f
 TITLE: Ring closure of N-alkoxalyl- β -anilinopropionic acids
 AUTHOR(S): Southwick, Philip L.; Seivard, Louis L.
 SOURCE: Journal of the American Chemical Society (1949), 71, 2532-8
 CODEN: JACSAT; ISSN: 0002-7863
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 OTHER SOURCE(S): CASREACT 43:46441
 AB KO2CCO2Me and SOCl2 (1 mol. each) give 63% MeO2CCOCl (I); EtO2CCOCl (II) results in 59% yield. PhNH2 (3 mols.) in 75 ml. AcOH, treated (1 hr.) with 3 mols. CH2:CHCO2Me, gives 57% PhNHCH2CH2CO2Me; KOH in MeOH gives 65% of the acid (III). PhNHCHPhCH2CO2H and twice its weight of I, heated 0.5 hr. on the steam bath, give 85% N-methoxalyl- β -anilino- β -phenylpropionic acid (IV), m. 127-8° (m.ps. corrected) (Me ester, m. 75-7°, 83%); N-ethoxalyl homolog (V), m. 111-13°, 78%. N-Ethoxalyl- β -anilinopropionic acid (VI), m. 91-2°, 58%; N-ethoxalyl- β -amino- β -phenylpropionic acid (VII), m. 116-18°, 43%. IV and an equal weight of I or II in 2 ml. CHCl3 per g. IV (dioxane can be used as the solvent), treated with C5H5N equal to the weight of the acid, kept 30 min. at room temperature, diluted with 5 vols. CHCl3, shaken 2 hrs. with an equal volume of H2O, and the CHCl3 layer extracted with excess 5% NaHCO3 and precipitated with 5% HCl, give 26% 1,5-diphenyl-2-keto-3-methoxy-3-pyrroline-4-carboxylic acid (VIII), m. 196-8°; Me ester, m. 128.5-30°; Et ester, m. 83-5°. V yields 32% of the 3-EtO analog (IX), m. 214-15°; Me ester (X), m. 91-2°; 3 g. V in 7

cc. Ac₂O and 7 g. C₅H₅N, heated 3 hrs. on the steam bath, gives 10% IX; no reaction occurs with Ac₂O or C₅H₅N alone. VI yields 15% 1-phenyl-2-keto-3-ethoxy-Δ³-pyrroline-4-carboxylic acid (XI), m. 189-91°; Me ester (XII), m. 75.5-7°. III and II in the presence of C₅H₅N give XI; in the absence of C₅H₅N, the product is VI. PhCH:NPh and MeO₂CCOCH₂CO₂Et give 66% Me 1,5-diphenyl-2,3-pyrrolidinedione-4-carboxylate (XIII), m. 201-3°; MeCHN₂ gives the Et ester. PhNHCH₂CH₂CO₂Me (7.2 g.) and 4.8 g. (CO₂Me)₂ in 50 ml. ether, treated (15 min.) with 2.5 g. MeONa in 50 ml. ether and refluxed 2 hrs., give 38% Me 1-phenyl-2,3-pyrrolidinedione-4-carboxylate, m. 185-7°; MeCHN₂ gives XII. The Et ester corresponding to XIII and CH₂N₂ give the Et ester of VIII. A mechanism is proposed for the ring closure reaction which relates it to the Perkin reaction and to the Claisen condensation.

IT 873399-08-7, 3-Pyrrolidinecarboxylic acid, 4,5-dioxo-1,2-diphenyl-
(esters)
RN 873399-08-7 CAPLUS
CN 3-Pyrrolidinecarboxylic acid, 4,5-dioxo-1,2-diphenyl- (CA INDEX NAME)



L3 ANSWER 61 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1947:1129 CAPLUS

DOCUMENT NUMBER: 41:1129

ORIGINAL REFERENCE NO.: 41:213h-i,214a

TITLE: Pharmacological activity of basic alkyl esters of substituted pyrrolidine dicarboxylic acids. II. Action on intestine, uterus, and blood pressure

AUTHOR(S): Loomis, Ted. A.; Schaffer, Norwood K.

CORPORATE SOURCE: Yale Univ.

SOURCE: Yale Journal of Biology and Medicine (1946), 18, 171-84

CODEN: YJBMAU; ISSN: 0044-0086

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB Fourteen of these compds. II, III, IV, V, VI, VII, VIII, X, XI, XII, XIII, XIV, XV, and XVI produced a spasmodic response in the circular muscle of the intact duodenum of the cat. The response of 15 mg./kg. of the most active was equivalent to 2 mg./kg. of BaCl₂. I, II, III, IV, V, VI, VIII, IX, XIV, XV, and XVI produced a spasmodic response in the intact uterus of the cat. All compds. caused fall in arterial blood pressure. VII, IX, XI, XII, XIII, and XVI were very toxic, 10 mg./kg. causing a 100% fall in blood pressure and heart rate.

IT 859957-82-7P, 2,5-Pyrrolidinedicarboxylic acid, 1-phenyl-, bis(2-diethylaminoethyl) and bis(3-diethylaminopropyl) esters 860360-52-7P, 2,5-Pyrrolidinedicarboxylic acid, 1-[2,4-xyllyl]-, bis(2-diethylaminoethyl) esters 860360-56-1P, 2,5-Pyrrolidinedicarboxylic acid, 1-o-tolyl-, bis(2-diethylaminoethyl) esters 860360-58-3P, 2,5-Pyrrolidinedicarboxylic acid, 1-m-tolyl-, bis(2-diethylaminoethyl) esters 874496-93-2P, 2,5-Pyrrolidinedicarboxylic acid, 1-p-tolyl-, 2-diethylaminoethyl ethyl ester 874496-98-7P, 2,5-Pyrrolidinedicarboxylic acid, 1-(p-chlorophenyl)-, bis(2-diethylaminoethyl) ester 875233-90-2P, 2,5-Pyrrolidinedicarboxylic acid, 1-cyclohexyl-, bis(3-

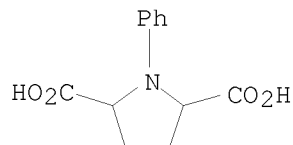
diethylaminopropyl) ester

RL: PREP (Preparation)

(preparation of)

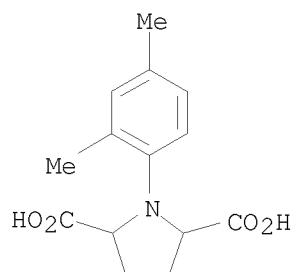
RN 859957-82-7 CAPLUS

CN 2,5-Pyrrolidinedicarboxylic acid, 1-phenyl- (CA INDEX NAME)



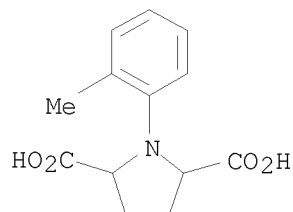
RN 860360-52-7 CAPLUS

CN 2,5-Pyrrolidinedicarboxylic acid, 1-(2,4-dimethylphenyl)- (CA INDEX NAME)



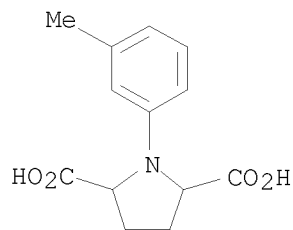
RN 860360-56-1 CAPLUS

CN 2,5-Pyrrolidinedicarboxylic acid, 1-(2-methylphenyl)- (CA INDEX NAME)



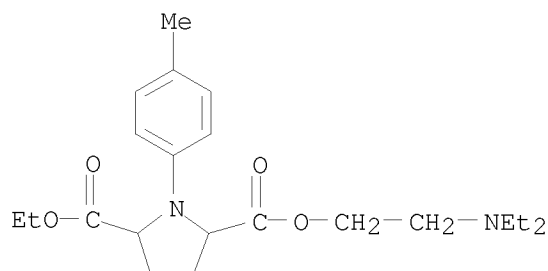
RN 860360-58-3 CAPLUS

CN 2,5-Pyrrolidinedicarboxylic acid, 1-(3-methylphenyl)- (CA INDEX NAME)

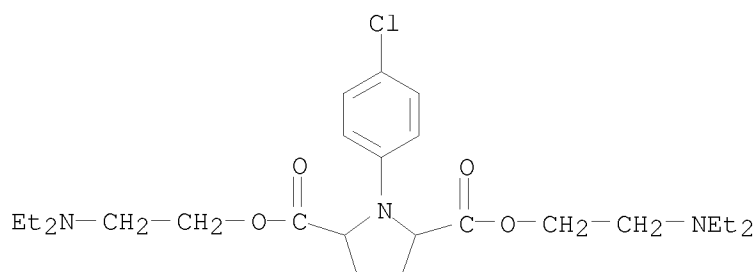


RN 874496-93-2 CAPLUS

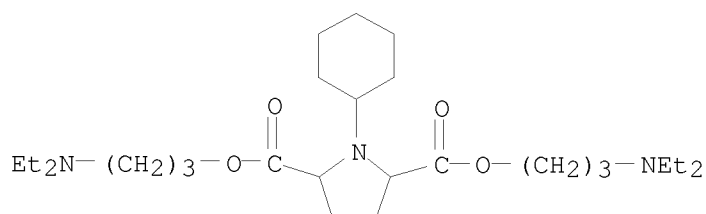
CN 2,5-Pyrrolidinedicarboxylic acid, 1-(4-methylphenyl)-,
2-[2-(diethylamino)ethyl] 5-ethyl ester (CA INDEX NAME)



RN 874496-98-7 CAPLUS
 CN 2,5-Pyrrolidinedicarboxylic acid, 1-(4-chlorophenyl)-,
 2,5-bis[2-(diethylamino)ethyl] ester (CA INDEX NAME)



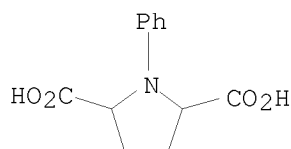
RN 875233-90-2 CAPLUS
 CN 2,5-Pyrrolidinedicarboxylic acid, 1-cyclohexyl-, 2,5-bis[3-(diethylamino)propyl] ester (CA INDEX NAME)



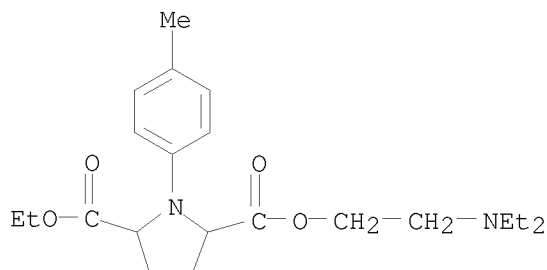
L3 ANSWER 62 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1947:1128 CAPLUS
 DOCUMENT NUMBER: 41:1128
 ORIGINAL REFERENCE NO.: 41:213f-h
 TITLE: Pharmacological activity of basic alkyl esters of substituted pyrrolidine dicarboxylic acids. I. Local anesthetic activity and toxicity
 AUTHOR(S): Schaffer, Norwood K.; Loomis, Ted A.
 CORPORATE SOURCE: Yale Univ.
 SOURCE: Yale Journal of Biology and Medicine (1946), 18, 157-64
 CODEN: YJBMAU; ISSN: 0044-0086
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 GI For diagram(s), see printed CA Issue.
 AB The local-anesthetic activity and toxicity were measured on the rabbit

cornea and by intraperitoneal injection in mice for 16 derivs. of 2,5-pyrrolidinedicarboxylic acid, (NR.CH(COOCH₂CH₂NEt₂).CH₂.CH₂.CHCOOCH₂CH₂NEt) where R = Et (I), MeOCH₂CH₂ (II), iso-Bu (III), hexyl (IV), benzyl (V), Ph (VI), o-tolyl (VII), m-tolyl (VIII), phenethyl (IX), p-ClC₆H₄ (X), 2,4-xylyl (XI), and 3,5-xylyl (XII); (NR.CH(COOCH₂CH₂CH₂NEt₂).CH₂.CH₂.CHCOOCH₂CH₂CH₂NEt₂) where R = Ph (XIII), cyclohexyl (XIV), and Bu (XV), and p-MeC₆H₄N.CH (COOEt).CH₂.CH₂.CHCOOCH₂CH₂NEt₂ (XVI). IV and V had the highest therapeutic indexes (3.4 times that of cocaine); VII, VIII, IX, XI, XII, and XVI had therapeutic indexes greater than cocaine. These were less toxic than cocaine.

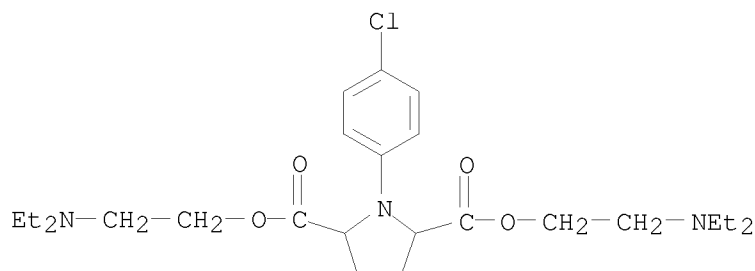
IT 859957-82-7P, 2,5-Pyrrolidinedicarboxylic acid, 1-phenyl-
 874496-93-2P, 2,5-Pyrrolidinedicarboxylic acid, 1-p-tolyl-,
 2-diethylaminoethyl ethyl ester 874496-98-7P,
 2,5-Pyrrolidinedicarboxylic acid, 1-(p-chlorophenyl)-,
 bis(2-diethylaminoethyl) ester 875233-90-2P,
 2,5-Pyrrolidinedicarboxylic acid, 1-cyclohexyl-, bis(3-diethylaminopropyl)
 ester
 RL: PREP (Preparation)
 (preparation of)
 RN 859957-82-7 CAPLUS
 CN 2,5-Pyrrolidinedicarboxylic acid, 1-phenyl- (CA INDEX NAME)



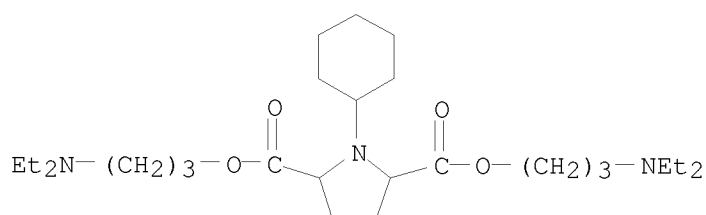
RN 874496-93-2 CAPLUS
 CN 2,5-Pyrrolidinedicarboxylic acid, 1-(4-methylphenyl)-,
 2-[2-(diethylamino)ethyl] 5-ethyl ester (CA INDEX NAME)



RN 874496-98-7 CAPLUS
 CN 2,5-Pyrrolidinedicarboxylic acid, 1-(4-chlorophenyl)-,
 2,5-bis[2-(diethylamino)ethyl] ester (CA INDEX NAME)



RN 875233-90-2 CAPLUS
 CN 2,5-Pyrrolidinedicarboxylic acid, 1-cyclohexyl-, 2,5-bis[3-(diethylamino)propyl] ester (CA INDEX NAME)

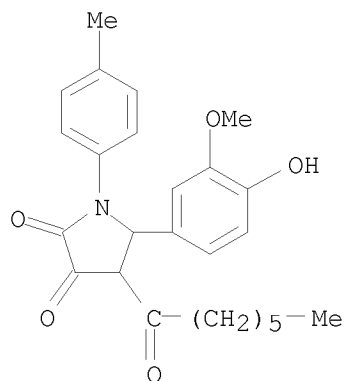


L3 ANSWER 63 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1946:27690 CAPLUS
 DOCUMENT NUMBER: 40:27690
 ORIGINAL REFERENCE NO.: 40:5427c-i,5428a-b
 TITLE: Condensation products of α,γ -diketo acids and their esters
 AUTHOR(S): Keskin, Halit
 CORPORATE SOURCE: Chemical Inst. II, Univ. of Istanbul, Turk.
 SOURCE: Rev. faculte sci. univ. Istanbul (1946), 11A(No. 1/2), 1-23
 DOCUMENT TYPE: Journal
 LANGUAGE: French
 GI For diagram(s), see printed CA Issue.
 AB cf. C.A. 40, 1490.4,9 18226. To 1 g. enanthylpyruvic acid in 5 ml. EtOH was added a solution of 0.35 g. $\text{H}_2\text{NNH}_2\cdot\text{HCl}$, and then 1 g. Na_2CO_3 . The next day the solution was acidified with H_2SO_4 and extracted with Et₂O. The extract was dried over Na_2SO_4 and evaporated on a watch glass, yielding 0.9 g. of 5-hexylisoxazole-3-carboxylic acid (I). Recrystd. from H₂O or petr. ether, the white product m. 104-5°. The 5-octyl derivative, prepared similarly from nonanoylpyruvic acid, m. 101-2°. Neither of the condensation products in alc. gives a color reaction with FeCl_3 . Both are monobasic, as shown by titration with NaOH. The Et esters of α,γ -diketo acids, condensed simultaneously with aromatic amines, RNH_2 , and aldehydes, $\text{R}'\text{CHO}$, yield 4,5-diketopyrrolidines consisting of an equilibrium mixture of the keto (II) and enol (III) forms.
 The enolization does not take place in the ring, as suggested by Schiff and Gigli (Ber. 31, 1307(1898)), but in the side chain. 1-p-Tolyl-2-phenyl-3-propionyl-4,5-diketopyrrolidine has been prepared by adding 0.9 ml. $\text{EtCOCH}_2\text{COCO}_2\text{Et}$ and 0.5 ml. of BzH to 0.5 g. p-toluidine in 5 ml. of C_6H_6 . After 2 days, the crystals were collected and washed with a little EtOH, yielding 1.3 g. Recrystd. from EtOH, the white crystals m. 222-4°.

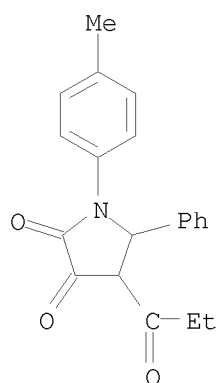
The following derivs. of 4,5-diketopyrrolidine were made similarly:
 1-phenyl-2-(p-methoxyphenyl)-3-butyryl, white crystals, m. 206-7°;
 1-p-tolyl-2-(p-methoxyphenyl)-3-butyryl, white crystals, m.
 189-90°; 1-phenyl-2-(p-methoxyphenyl)-3-isovaleryl, m.
 216-17°; 1-p-tolyl-2-(p-methoxyphenyl)-3-isovaleryl, m.
 200-1°; 1-phenyl-2-(p-methoxyphenyl)-3-caproyl, white crystals, m.
 182°; 1-p-tolyl-2-(p-methoxyphenyl)-3-caproyl, white crystals, m.
 190-1°; 1,2-diphenyl-3-enanthyl, m. 182°;
 1-p-tolyl-2-phenyl-3-enanthyl, white crystals, m. 186°;
 1-phenyl-2-(p-methoxyphenyl)-3-enanthyl, m. 173°;
 1-p-tolyl-2-(p-methoxyphenyl)-3-enanthyl, m. 206-7°;
 1-phenyl-2-(p-dimethylaminophenyl)-3-enanthyl, pale yellow, m.
 180-1°; 1-p-tolyl-2-(p-dimethylaminophenyl)-3-enanthyl, pale
 yellow, m. 232°; 1-phenyl-2-(4-hydroxy-3-methoxyphenyl)-3-enanthyl,
 white crystals, m. 204°; 1-p-tolyl-2-(4-hydroxy-3-methoxyphenyl)-3-
 enanthyl, m. 208°; 1-(1-naphthyl)-2-phenyl-3-enanthyl, m.
 194-5°; 1-(2-naphthyl)-2-phenyl-3-enanthyl, m. 192°;
 1,2-diphenyl-3-nonanoyl, m. 173°; 1-p-tolyl-2-phenyl-3-nonanoyl m.
 184°; 1-phenyl-2-(p-methoxyphenyl)-3-nonanoyl, m. 139°;
 1-p-tolyl-2-(p-methoxyphenyl)-3-nonanoyl, m. 171-2°;
 1-phenyl-2-(p-dimethylaminophenyl)-3-nonanoyl, pale yellow crystals, m.
 182-3°; 1-p-tolyl-2-(p-dimethylaminophenyl)-3-nonanoyl, yellow
 crystals, m. 189°; 1-m-tolyl-2-(4-hydroxy-3-methoxyphenyl)-3-
 nonanoyl, m. 168-9°; 1-(1-naphthyl)-2-phenyl-3-nonanoyl; white
 crystals, m. 175-6°; 1-(2-naphthyl)-2-phenyl-3-nonanoyl, white
 crystals, m. 182-3°; 1-phenyl-2-(p-methoxyphenyl)-3-decanoyl, m.
 140-1°; 1-p-tolyl-2-(p-methoxyphenyl)-3-decanoyl, m.
 149-50°; 1-phenyl-2-(p-methoxyphenyl)-3-dodecanoyl, m.
 115-17°; 1-p-tolyl-2-(p-methoxyphenyl)-3-dodecanoyl, m.
 142°. All these substituted diketopyrrolidines have 1 acid
 function, and give a blood-red color reaction with FeCl₃ in EtOH.

IT

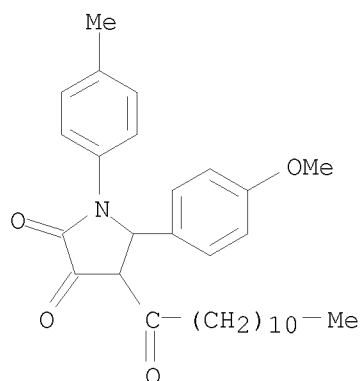
854896-66-5P, 2,3-Pyrrolidinedione, 4-enanthyl-5-(4-hydroxy-3-
 methoxyphenyl)-1-p-tolyl- 858273-78-6P, 2,3-Pyrrolidinedione,
 5-phenyl-4-propionyl-1-p-tolyl- 858274-03-0P,
 2,3-Pyrrolidinedione, 4-lauroyl-5-(p-methoxyphenyl)-1-p-tolyl-
 858274-04-1P, 2,3-Pyrrolidinedione, 4-lauroyl-5-(p-methoxyphenyl)-
 1-phenyl- 858274-22-3P, 2,3-Pyrrolidinedione,
 4-caproyl-5-(p-methoxyphenyl)-1-p-tolyl- 858274-23-4P,
 2,3-Pyrrolidinedione, 4-caproyl-5-(p-methoxyphenyl)-1-phenyl-
 858274-24-5P, 2,3-Pyrrolidinedione, 4-butyryl-5-(p-methoxyphenyl)-
 1-p-tolyl- 858274-25-6P, 2,3-Pyrrolidinedione,
 4-butyryl-5-(p-methoxyphenyl)-1-phenyl- 861035-28-1P,
 2,3-Pyrrolidinedione, 4-isovaleryl-5-(p-methoxyphenyl)-1-p-tolyl-
 861035-30-5P, 2,3-Pyrrolidinedione, 4-isovaleryl-5-(p-
 methoxyphenyl)-1-phenyl- 861035-37-2P, 2,3-Pyrrolidinedione,
 4-enanthyl-5-phenyl-1-p-tolyl- 861035-39-4P,
 2,3-Pyrrolidinedione, 4-enanthyl-1-[2-naphthyl]-5-phenyl-
 861035-41-8P, 2,3-Pyrrolidinedione, 4-enanthyl-1-[1-naphthyl]-5-
 phenyl- 861035-43-0P, 2,3-Pyrrolidinedione, 4-enanthyl-5-(p-
 methoxyphenyl)-1-p-tolyl- 861035-45-2P, 2,3-Pyrrolidinedione,
 4-enanthyl-5-(p-methoxyphenyl)-1-phenyl- 861035-47-4P,
 2,3-Pyrrolidinedione, 4-enanthyl-5-(4-hydroxy-2-methoxyphenyl)-1-phenyl-
 861035-49-6P, 2,3-Pyrrolidinedione, 4-enanthyl-1,5-diphenyl-
 861035-59-8P, 2,3-Pyrrolidinedione, 5-(p-dimethylaminophenyl)-4-
 enanthyl-1-p-tolyl- 861035-61-2P, 2,3-Pyrrolidinedione,
 5-(p-dimethylaminophenyl)-4-enanthyl-1-phenyl-
 RL: PREP (Preparation)
 (preparation of)
 RN 854896-66-5 CAPLUS
 CN 2,3-Pyrrolidinedione, 5-(4-hydroxy-3-methoxyphenyl)-1-(4-methylphenyl)-4-
 (1-oxoheptyl)- (CA INDEX NAME)



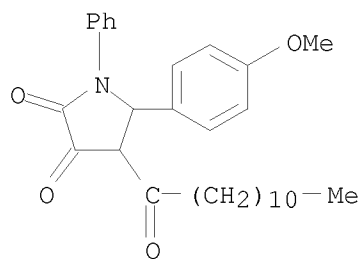
RN 858273-78-6 CAPLUS
 CN 2,3-Pyrrolidinedione, 1-(4-methylphenyl)-4-(1-oxopropyl)-5-phenyl- (CA INDEX NAME)



RN 858274-03-0 CAPLUS
 CN 2,3-Pyrrolidinedione, 5-(4-methoxyphenyl)-1-(4-methylphenyl)-4-(1-oxododecyl)- (CA INDEX NAME)

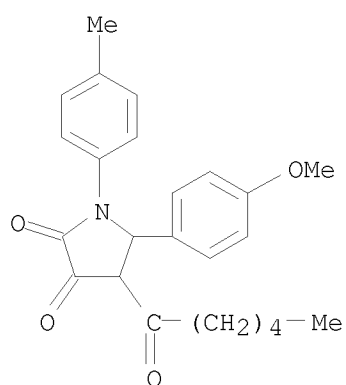


RN 858274-04-1 CAPLUS
 CN 2,3-Pyrrolidinedione, 5-(4-methoxyphenyl)-4-(1-oxododecyl)-1-phenyl- (CA INDEX NAME)



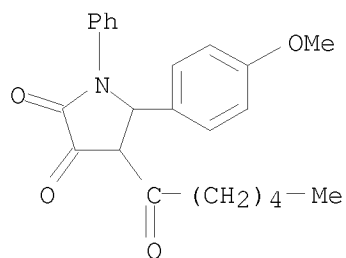
RN 858274-22-3 CAPLUS

CN 2,3-Pyrrolidinedione, 5-(4-methoxyphenyl)-1-(4-methylphenyl)-4-(1-oxohexyl)- (CA INDEX NAME)



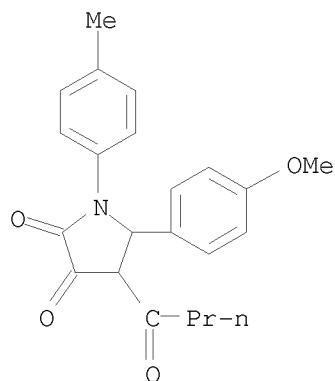
RN 858274-23-4 CAPLUS

CN 2,3-Pyrrolidinedione, 5-(4-methoxyphenyl)-4-(1-oxohexyl)-1-phenyl- (CA INDEX NAME)

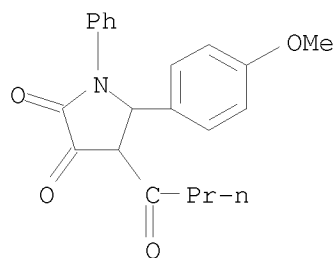


RN 858274-24-5 CAPLUS

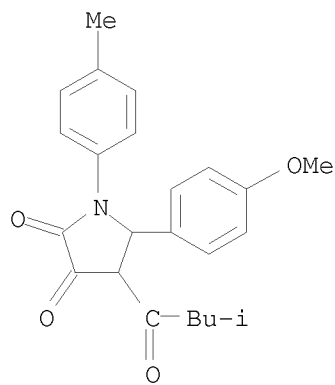
CN 2,3-Pyrrolidinedione, 5-(4-methoxyphenyl)-1-(4-methylphenyl)-4-(1-oxobutyl)- (CA INDEX NAME)



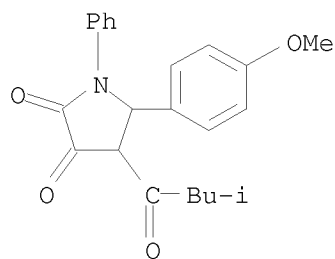
RN 858274-25-6 CAPLUS
 CN 2,3-Pyrrolidinedione, 5-(4-methoxyphenyl)-4-(1-oxobutyl)-1-phenyl- (CA INDEX NAME)



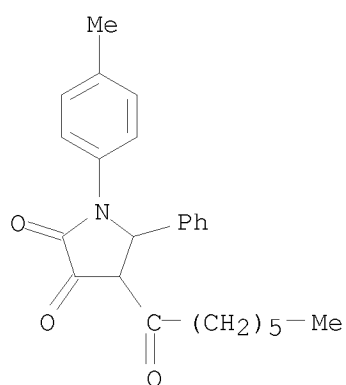
RN 861035-28-1 CAPLUS
 CN 2,3-Pyrrolidinedione, 5-(4-methoxyphenyl)-4-(3-methyl-1-oxobutyl)-1-(4-methylphenyl)- (CA INDEX NAME)



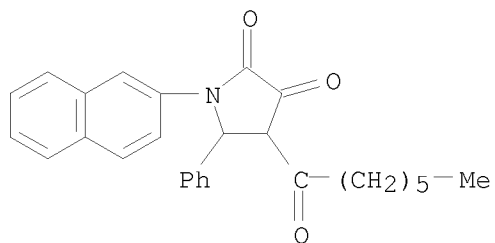
RN 861035-30-5 CAPLUS
 CN 2,3-Pyrrolidinedione, 5-(4-methoxyphenyl)-4-(3-methyl-1-oxobutyl)-1-phenyl- (CA INDEX NAME)



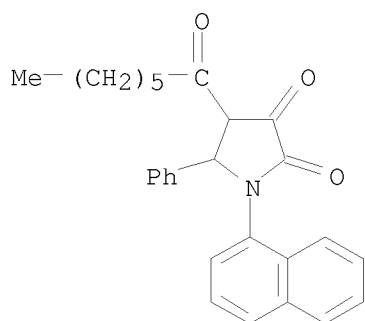
RN 861035-37-2 CAPLUS
 CN 2,3-Pyrrolidinedione, 1-(4-methylphenyl)-4-(1-oxoheptyl)-5-phenyl- (CA
 INDEX NAME)



RN 861035-39-4 CAPLUS
 CN 2,3-Pyrrolidinedione, 1-(2-naphthalenyl)-4-(1-oxoheptyl)-5-phenyl- (CA
 INDEX NAME)

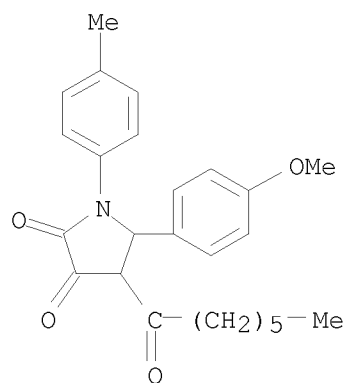


RN 861035-41-8 CAPLUS
 CN 2,3-Pyrrolidinedione, 1-(1-naphthalenyl)-4-(1-oxoheptyl)-5-phenyl- (CA
 INDEX NAME)



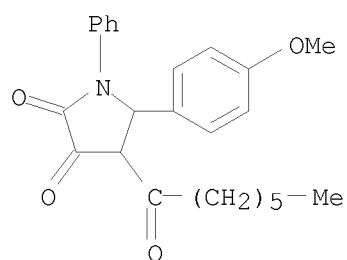
RN 861035-43-0 CAPLUS

CN 2,3-Pyrrolidinedione, 5-(4-methoxyphenyl)-1-(4-methylphenyl)-4-(1-oxoheptyl)- (CA INDEX NAME)



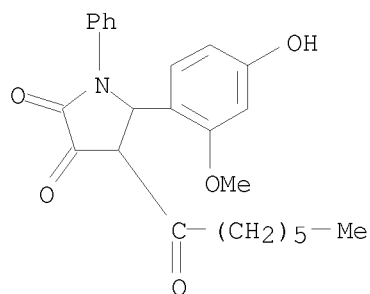
RN 861035-45-2 CAPLUS

CN 2,3-Pyrrolidinedione, 5-(4-methoxyphenyl)-4-(1-oxoheptyl)-1-phenyl- (CA INDEX NAME)



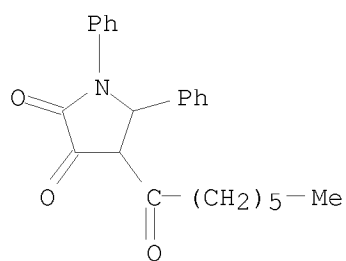
RN 861035-47-4 CAPLUS

CN 2,3-Pyrrolidinedione, 5-(4-hydroxy-2-methoxyphenyl)-4-(1-oxoheptyl)-1-phenyl- (CA INDEX NAME)



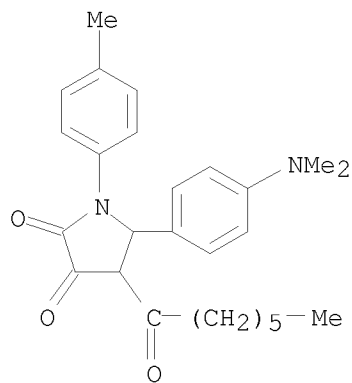
RN 861035-49-6 CAPLUS

CN 2,3-Pyrrolidinedione, 4-(1-oxoheptyl)-1,5-diphenyl- (CA INDEX NAME)



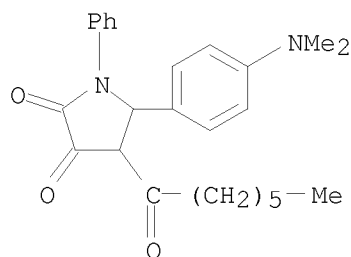
RN 861035-59-8 CAPLUS

CN 2,3-Pyrrolidinedione, 5-[4-(dimethylamino)phenyl]-1-(4-methylphenyl)-4-(1-oxoheptyl)- (CA INDEX NAME)



RN 861035-61-2 CAPLUS

CN 2,3-Pyrrolidinedione, 5-[4-(dimethylamino)phenyl]-4-(1-oxoheptyl)-1-phenyl- (CA INDEX NAME)



L3 ANSWER 64 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN

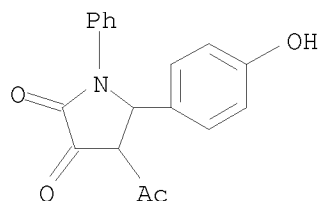
ACCESSION NUMBER: 1939:55382 CAPLUS
 DOCUMENT NUMBER: 33:55382
 ORIGINAL REFERENCE NO.: 33:7963b-h
 TITLE: Pyrrolidine derivatives
 INVENTOR(S): Dohrn, Max; Nahme, Hans
 PATENT ASSIGNEE(S): Schering A.-G.
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 678152		19390711	DE 1937-SC114287	19371119

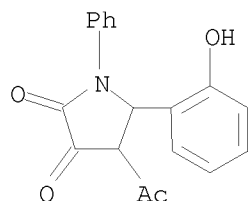
AB Substitution products of 4,5-diketo-pyrrolidine (I) are obtained by condensing an easily saponifiable derivative of a hydroxybenzaldehyde, e. g., an acyloxybenzaldehyde or a hydroxybenzaldehyde alkyl-carbonic acid ester, with a primary aromatic, alicyclic or heterocyclic amine and an α -keto carboxylic ester, e. g., an oxalacetic or acylpyruvic ester. The products may then be treated to remove the easily saponifiable group. In a typical example, p-OHCC6H4OCOOMe, PhNH₂ and AcCH₂COCOOEt are allowed to stand in benzene solution to yield 1-phenyl-3-acetyl-2-(4'-carbomethoxyoxyphenyl)-I, m. 205°, which yields 1-phenyl-3-acetyl-2-(4'-hydroxyphenyl)-I, m. 244-6°, when warmed with caustic alkali solution. Similarly, p-OHCC6H4OCOOMe, PhNH₂ and PhCOCH₂COCOOEt yield 1-phenyl-3-benzoyl-2-(4'-carbomethoxyoxyphenyl)-I, m. 238°, which yields 1-phenyl-3-benzoyl-2-(4'-hydroxyphenyl)-I, m. 248°, when saponified, and p-OHCC6H4OCOOMe, PhNH₂ and EtO-OCCOCH₂COCOOEt yield 1-phenyl-3-carbomethoxy-2-(4'-carbomethoxyoxyphenyl)-I, m. 168-70°, which yields 1-phenyl-2-(4'-hydroxyphenyl)-I-3-carboxylic acid, decomposing 240°, when saponified. Examples are given also of the preparation of (a) 1-(4'-carbomethoxyoxyphenyl)-3-acetyl-2-(4'-carbomethoxyoxyphenyl)-I, m. 223°, which yields 1-(4'-carboxyphenyl)-3-acetyl-2-(4'-hydroxyphenyl)-I, m. 265°, when saponified, (b) 1-(4'-dimethylaminophenyl)-3-acetyl-2-(4'-carbomethoxyoxyphenyl)-I, m. 139-42°, and the corresponding 2-(4'-hydroxyphenyl) compound, m. 243°, (c) 1-(4'-iodophenyl)-3-acetyl-2-(4'-carbomethoxyoxyphenyl)-I, m. 225°, and the corresponding 2-(4'-hydroxyphenyl) compound, m. 255°, (d) 1-(3',4',5'-triiodophenyl)-3-acetyl-2-(4'-carbomethoxyoxyphenyl)-I, m. 230° (decomposition), and the corresponding 2-(4'-hydroxyphenyl) compound, m. 263° (decomposition), (e) 1-(2'-butyloxy - 5' - pyridyl) - 3 - acetyl - 2 - (4' - carbomethoxyoxyphenyl)-I, m. 100°, and the corresponding 2-(4'-hydroxyphenyl) compound, m. 220°, (f) 1-(6'-quinolyl)-3-acetyl-2-(4'-carbomethoxyoxyphenyl)-I, decomposing above 270°, and the corresponding 2-(4'-hydroxyphenyl) compound, m. above 260° (decomposition), (g) 1-cyclohexyl-3-acetyl-2-(4'-carbomethoxyoxyphenyl)-I, m. 195-6°, and the corresponding

2-(4'-hydroxyphenyl) compound, m. 239°, (h) 1-phenyl-3-acetyl-2-(2'carboethoxyoxyphenyl)-I, m. 171°, and the corresponding 2-(2'-hydroxyphenyl) compound, m. 198-200°, (i) 1-phenyl-3-acetyl-2-(3'-carbomethoxyoxyphenyl)-I, m. 191°, and the corresponding 2-(3'-hydroxyphenyl) compound, m. 183° (j) 1-phenyl-3-acetyl-2-(4'-acetoxyphenyl)-I, m. 205-6°, and the corresponding 2-(4'-hydroxyphenyl) compound, (k) 1-phenyl-3-acetyl-2-(4'-benzyloxyphenyl)-I, m. 236-7°. The products are useful as drugs or intermediates for drugs.

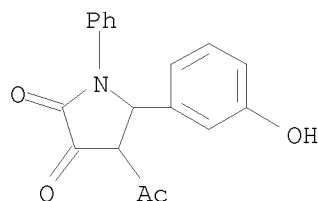
IT 852058-50-5, 2,3-Pyrrolidinedione, 4-acetyl-5-[p-hydroxyphenyl]-1-phenyl- 858274-45-0, 2,3-Pyrrolidinedione, 4-acetyl-5-[o-hydroxyphenyl]-1-phenyl- 858274-47-2, 2,3-Pyrrolidinedione, 4-acetyl-5-[m-hydroxyphenyl]-1-phenyl- (and esters)
 RN 852058-50-5 CAPLUS
 CN 2,3-Pyrrolidinedione, 4-acetyl-5-(4-hydroxyphenyl)-1-phenyl- (CA INDEX NAME)



RN 858274-45-0 CAPLUS
 CN 2,3-Pyrrolidinedione, 4-acetyl-5-(2-hydroxyphenyl)-1-phenyl- (CA INDEX NAME)



RN 858274-47-2 CAPLUS
 CN 2,3-Pyrrolidinedione, 4-acetyl-5-(3-hydroxyphenyl)-1-phenyl- (CA INDEX NAME)

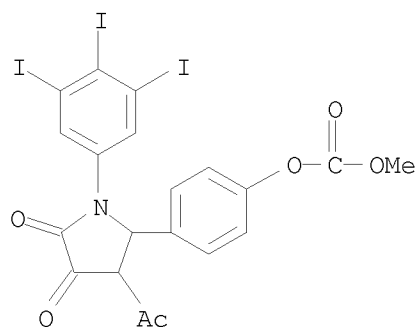


IT 858274-37-0P, 2,3-Pyrrolidinedione, 4-acetyl-5-(p-hydroxyphenyl)-1-(3,4,5-triiodophenyl)-, methyl carbonate 858274-39-2P, 2,3-Pyrrolidinedione, 4-acetyl-5-(p-hydroxyphenyl)-1-(3,4,5-triiodophenyl)- 858274-42-7P, 2,3-Pyrrolidinedione, 4-acetyl-5-(p-hydroxyphenyl)-1-(6-quinolyl)-, methyl carbonate 858274-43-8P, 2,3-Pyrrolidinedione, 4-acetyl-5-(p-hydroxyphenyl)-1-(6-quinolyl)-

858274-49-4P, 2,3-Pyrrolidinedione, 4-acetyl-5-(p-hydroxyphenyl)-1-(p-iodophenyl)-, methyl carbonate 861035-81-6P,
 2,3-Pyrrolidinedione, 4-acetyl-5-(p-hydroxyphenyl)-1-(p-iodophenyl)- 861035-84-9P, 2,3-Pyrrolidinedione, 4-acetyl-1-(p-dimethylaminophenyl)-5-(p-hydroxyphenyl)-, methyl carbonate 861035-85-0P, 2,3-Pyrrolidinedione, 4-acetyl-1-(p-dimethylaminophenyl)-5-(p-hydroxyphenyl)- 861035-86-1P,
 2,3-Pyrrolidinedione, 4-acetyl-1-cyclohexyl-5-(p-hydroxyphenyl)-, methyl carbonate 861035-87-2P, 2,3-Pyrrolidinedione, 4-acetyl-1-cyclohexyl-5-(p-hydroxyphenyl)- 861035-88-3P,
 2,3-Pyrrolidinedione, 4-acetyl-1-(p-carboxyphenyl)-5-(p-hydroxyphenyl)-, Et ester methyl carbonate 861035-89-4P, 2,3-Pyrrolidinedione, 4-acetyl-1-(p-carboxyphenyl)-5-(p-hydroxyphenyl)- 861035-90-7P,
 2,3-Pyrrolidinedione, 4-acetyl-1-(6-butoxy-3-pyridyl)-5-(p-hydroxyphenyl)-, methyl carbonate 861035-91-8P, 2,3-Pyrrolidinedione, 4-acetyl-1-(6-butoxy-3-pyridyl)-5-(p-hydroxyphenyl)- 861035-92-9P
 RL: PREP (Preparation)
 (preparation of)

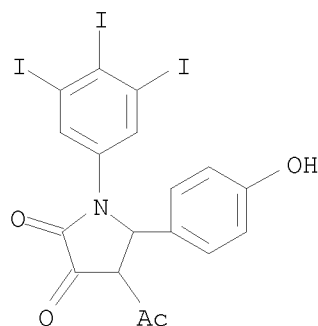
RN 858274-37-0 CAPLUS

CN 2,3-Pyrrolidinedione, 4-acetyl-5-(p-hydroxyphenyl)-1-(3,4,5-triiodophenyl)-, methyl carbonate (4CI) (CA INDEX NAME)



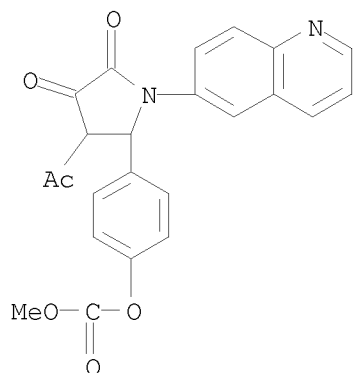
RN 858274-39-2 CAPLUS

CN 2,3-Pyrrolidinedione, 4-acetyl-5-(4-hydroxyphenyl)-1-(3,4,5-triiodophenyl)- (CA INDEX NAME)

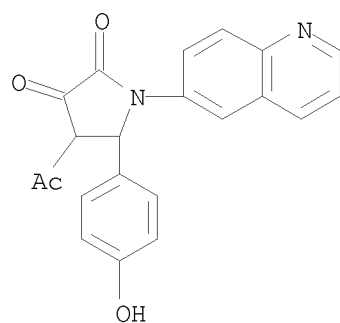


RN 858274-42-7 CAPLUS

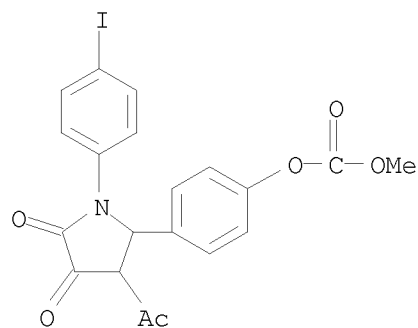
CN 2,3-Pyrrolidinedione, 4-acetyl-5-(p-hydroxyphenyl)-1-(6-quinolyl)-, methyl carbonate (4CI) (CA INDEX NAME)



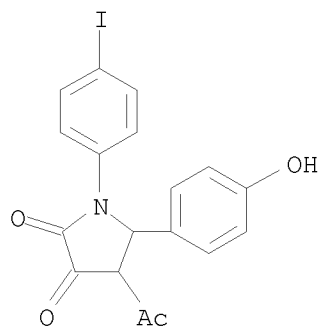
RN 858274-43-8 CAPLUS
 CN 2,3-Pyrrolidinedione, 4-acetyl-5-(4-hydroxyphenyl)-1-(6-quinolinyl)- (CA INDEX NAME)



RN 858274-49-4 CAPLUS
 CN 2,3-Pyrrolidinedione, 4-acetyl-5-(p-hydroxyphenyl)-1-(p-iodophenyl)-, methyl carbonate (4CI) (CA INDEX NAME)

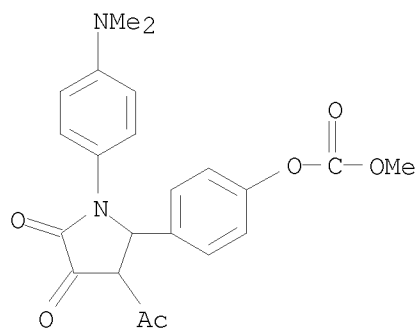


RN 861035-81-6 CAPLUS
 CN 2,3-Pyrrolidinedione, 4-acetyl-5-(4-hydroxyphenyl)-1-(4-iodophenyl)- (CA INDEX NAME)



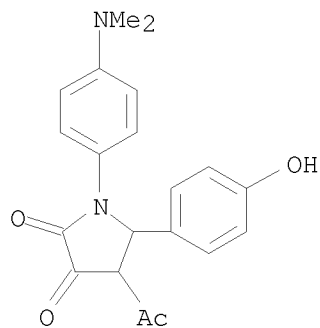
RN 861035-84-9 CAPLUS

CN 2,3-Pyrrolidinedione, 4-acetyl-1-(p-dimethylaminophenyl)-5-(p-hydroxyphenyl)-, methyl carbonate (4CI) (CA INDEX NAME)



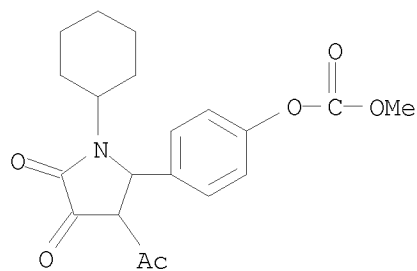
RN 861035-85-0 CAPLUS

CN 2,3-Pyrrolidinedione, 4-acetyl-1-[4-(dimethylamino)phenyl]-5-(4-hydroxyphenyl)- (CA INDEX NAME)



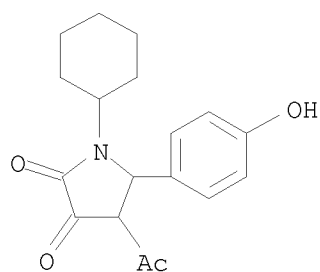
RN 861035-86-1 CAPLUS

CN 2,3-Pyrrolidinedione, 4-acetyl-1-cyclohexyl-5-(p-hydroxyphenyl)-, methyl carbonate (4CI) (CA INDEX NAME)



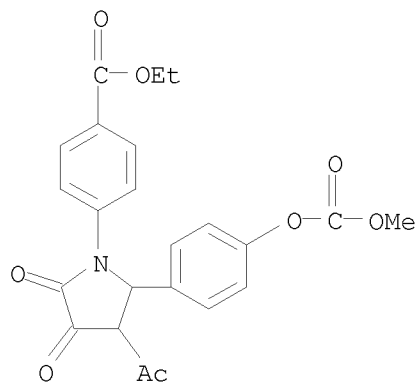
RN 861035-87-2 CAPLUS

CN 2,3-Pyrrolidinedione, 4-acetyl-1-cyclohexyl-5-(4-hydroxyphenyl)- (CA
INDEX NAME)



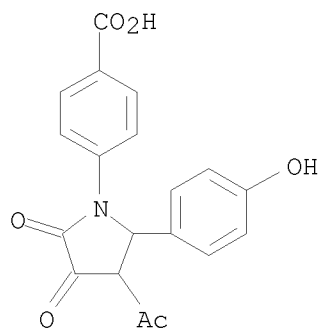
RN 861035-88-3 CAPLUS

CN INDEX NAME NOT YET ASSIGNED



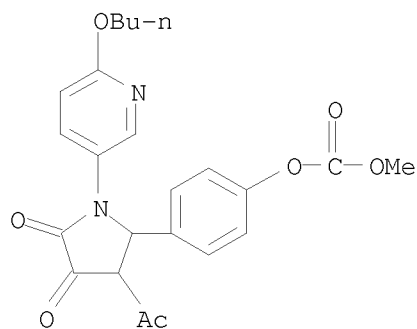
RN 861035-89-4 CAPLUS

CN INDEX NAME NOT YET ASSIGNED



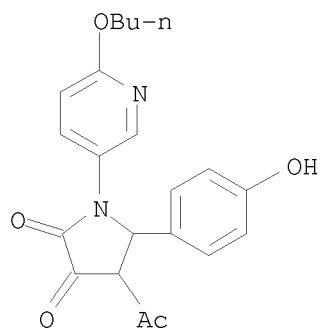
RN 861035-90-7 CAPLUS

CN 2,3-Pyrrolidinedione, 4-acetyl-1-(6-butoxy-3-pyridyl)-5-(p-hydroxyphenyl)-
, methyl carbonate (4CI) (CA INDEX NAME)



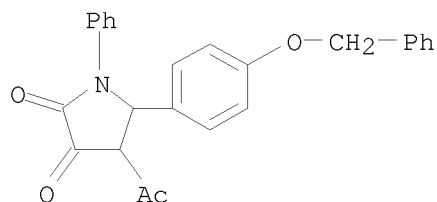
RN 861035-91-8 CAPLUS

CN 2,3-Pyrrolidinedione, 4-acetyl-1-(6-butoxy-3-pyridinyl)-5-(4-hydroxyphenyl)- (CA INDEX NAME)



RN 861035-92-9 CAPLUS

CN 2,3-Pyrrolidinedione, 4-acetyl-1-phenyl-5-[4-(phenylmethoxy)phenyl]- (CA INDEX NAME)



L3 ANSWER 65 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1938:30152 CAPLUS

DOCUMENT NUMBER: 32:30152

ORIGINAL REFERENCE NO.: 32:4166d-h

TITLE: Quinoline derivatives. III

AUTHOR(S): Ghosh, Tejendra N.

SOURCE: J. Indian Chem. Soc. (1937), 14, 713-16

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. C. A. 31, 7431.8. In that the therapeutic value of ichthyol oils has been attributed to the presence of alkylthiophenes and the replacement of the Ph group in the cinchophen mol. by the thiophene radical results in a product with marked antiphlogistic and analgesic properties it has seemed of interest to synthesize a compound in which the thiophene ring is fused with the quinoline residue. A mixture of 10.4 g. of Et 3,4-dihydroxythiophene-2,5-dicarboxylate and 7.5 g. PhNH₂ was heated on an oil bath for 30 min. and at 170-5° for 2.5 hrs. The product was triturated and washed with alc. and crystallized from dilute pyridine, yielding 8.5 g. of 2,5-diphenylcarbamido-3,4-dihydroxythiophene (I), C₁₈H₁₄N₂O₄S, m. 292-3° (decomposition). I (6 g.) was heated with 30 cc. concentrated H₂SO₄ for 3 hrs. at 100° and the cooled reaction mixture was poured onto ice, treated with excess Na₂CO₃, filtered and acidified. The greenish white amorphous solid was recrystd. from hot H₂O and gave 1.5 g. of 4-hydroxythiophene-2,3-(3',4')-2'-hydroxyquinolinesulfonic acid, C₁₁H₇N₂O₅S₂, m. above 310°, forming HBr and HCl salts, both m. above 300°. Attempts were made to condense Et 1-N-phenyl-3,4-dihydroxypyrrolidine-2,5-dicarboxylate with PhNH₂ but no reaction was observed. Following the work of Narang and Ray (C. A. 25, 3342) on the synthesis of glyoxalinoquinolines as antimalarials, 13.2 g. of 2-methylbenziminazole was condensed with 7.3 g. (CO₂Et)₂ in the presence of 2.3 g. Na in 100 cc. absolute alc. The mass was diluted with H₂O and extracted

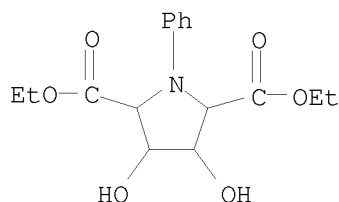
with Et₂O. Acidification of the aqueous solution with excess dilute HCl and recrystn. of the washed precipitate from hot H₂O gave 3 g. of 1,4-dibenziminazolylbiacetyl (II), C₁₈H₁₄N₄O₂, m. above 300°. Synthesis of bis(benziminazolylquinoline) derivs. by condensation of II with o-O₂NC₆H₄CHO in the presence of Ac₂O and fused NaOAc and in pyridine in the presence of piperidine was not achieved even on continued refluxing.

IT 861035-94-1P, 2,5-Pyrrolidinedicarboxylic acid, 3,4-dihydroxy-1-phenyl-, diethyl ester

RL: PREP (Preparation)
(preparation of)

RN 861035-94-1 CAPLUS

CN 2,5-Pyrrolidinedicarboxylic acid, 3,4-dihydroxy-1-phenyl-, 2,5-diethyl ester (CA INDEX NAME)



L3 ANSWER 66 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1932:18264 CAPLUS

DOCUMENT NUMBER: 26:18264

ORIGINAL REFERENCE NO.: 26:1928a-e

TITLE: Pyrazopyrrolidones

AUTHOR(S): Dohrn, M.; Thiele, A.

SOURCE: Berichte der Deutschen Chemischen Gesellschaft
[Abteilung] B: Abhandlungen (1931), 64B, 2863-5
CODEN: BDCBAD; ISSN: 0365-9488

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

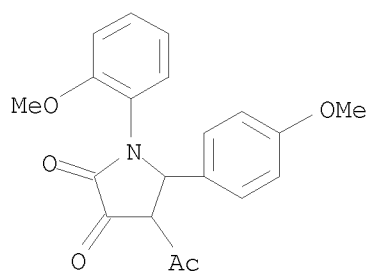
AB By condensation of primary or secondary amines with an aldehyde and α,γ -diketonic acid mixture Schiff obtained diketopyrrolidines (I) with an RCO group on C atom 3. From the I there can be obtained, through ketonization of the enolic group in position 4, 4-hydrazones which are capable of again forming a ring, with the 3-RCO group, yielding a bicyclic system (II) of two 5-membered rings with two C atoms in common. This 2nd ring closure does not take place when the substituent on C atom 3 is RO₂C instead of RCO. 2-Phenyl-3-acetyl-4,5-diketopyrrolidine, from BzH and saturated alc. NH₃ in benzene with AcCH₂COCO₂Et, m. 195-6°, gives a wine-red color with alc. FeCl₃; phenylhydrazone, m. 217°. The latter, boiled in alc. containing a little concentrated H₂SO₄, condenses to 2,4-diphenyl-3-methylpyrazo-6-pyrrolidone, m. 214-5°. In the same way were obtained the following addnl. 3-methylpyrazo-6-pyrrolidones: 1,4-dimethyl-2-phenyl, m. 250-5°; 2-piperonyl-4-phenyl, m. 216-7°; 1,2,4-triphenyl, m. 158-9°; 1-m-tolyl-2-p-methoxyphenyl-4-phenyl, m. 167-9°; 1-o-methoxyphenyl-2-p-methoxyphenyl-4-phenyl, m. 161-3°; 1,2-bis(p-methoxyphenyl)-4-phenyl, m. 162-40°; 1,2,3,4-tetraphenylpyrazo-6-pyrrolidone, m. 195-7°. These compds. were prepared from hydrazones of the following 3-acetyl-4,5-diketopyrrolidines: 1-methyl-2-phenyl, m. 215-60° (methylhydrazone, m. 204-5°); 2-piperonyl, m. 158-9°; 1,2-di-Ph, m. 229-310 (p-tolylhydrazone, m. 218° (decomposition)); 1-m-tolyl-2-P-methoxyphenyl, m. 186-8°; 1-o-methoxyphenyl-2-p-methoxyphenyl, turns brown 210°, m. 218-20°; 1,2-bis(p-methoxyphenyl), m. 163-40°.

IT 856099-62-2P, 2,3-Pyrrolidinedione, 4-acetyl-1-o-anisyl-5-p-anisyl-858450-37-0P, 2,3-Pyrrolidinedione, 4-acetyl-1,5-diphenyl-, 3-p-tolylhydrazone 858450-38-1P, 2,3-Pyrrolidinedione, 4-acetyl-1,5-di-p-anisyl- 858450-39-2P, 2,3-Pyrrolidinedione, 4-acetyl-5-p-anisyl-1-m-tolyl-

RL: PREP (Preparation)
(preparation of)

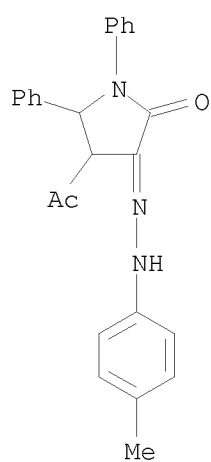
RN 856099-62-2 CAPLUS

CN 2,3-Pyrrolidinedione, 4-acetyl-1-(2-methoxyphenyl)-5-(4-methoxyphenyl)-
(CA INDEX NAME)



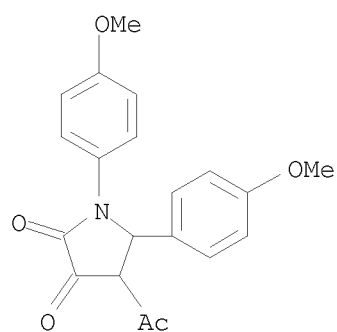
RN 858450-37-0 CAPLUS

CN 2,3-Pyrrolidinedione, 4-acetyl-1,5-diphenyl-, 3-[2-(4-methylphenyl)hydrazone] (CA INDEX NAME)



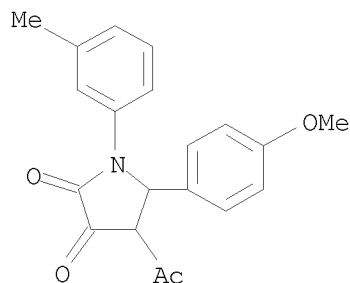
RN 858450-38-1 CAPLUS

CN 2,3-Pyrrolidinedione, 4-acetyl-1,5-bis(4-methoxyphenyl)- (CA INDEX NAME)



RN 858450-39-2 CAPLUS

CN 2,3-Pyrrolidinedione, 4-acetyl-5-(4-methoxyphenyl)-1-(3-methylphenyl)- (CA INDEX NAME)



L3 ANSWER 67 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1925:3519 CAPLUS

DOCUMENT NUMBER: 19:3519

ORIGINAL REFERENCE NO.: 19:503e-i

TITLE: Interaction between ethyl ethylidenemalonate and anilinophenylacetonitrile

AUTHOR(S): Higginbotham, Lucy; Lapworth, Arthur; Simpson, Charles

SOURCE: Journal of the Chemical Society, Transactions (1924), 125, 2339-44

CODEN: JCHTA3; ISSN: 0368-1645

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. Clarke and Lapworth, C. A. 1, 2116. The condensation of 25.5 g. PhCH(CN)NHPH and 22.8 g. MeCH:C(CO₂Et)₂ in ice-cold EtOH by adding dropwise 6.85 g. KOH in an equal weight of H₂O gives 19.5 g. of a precipitate

A, 5.8 g. of a yellow resin (after adding H₂O) and, after heating on the H₂O bath for several hrs., 10.5 g. of a resinous acid B. A was probably the K derivative of PhC[CHMeCH(CO₂Et)₂](CN)NHPH; boiled with 25% aqueous NaOH the steam

contained PhNH₂ and EtOH and the alkaline residue contained cyanide. With concentrated EtOH-KOH, NH₃ is evolved and cyanide formed; the Et₂O-soluble acids

consisted almost wholly of I, below. Heated in aqueous Me₂CO or in dilute AcOH,

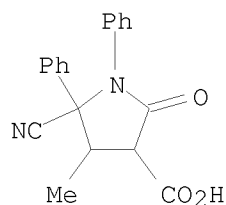
10 g. A gave about 6 g. Et 5-cyano-2-keto-1,5-diphenyl-4-methylpyrrolidine-3-carboxylate, m. 99°; it is repptd. unchanged from cold concentrated H₂SO₄; on heating it chars. It is not changed by boiling with dilute HCl but EtOH-H₂SO₄ gives BzOEt. The free acid was obtained only as a resin (B above), softens 40° and completely liquid at 65°. Heating 2 hrs. with 50% KOH gives I. Boiling with HCl gives 5-cyano-2-keto-1,5-diphenyl-4-methylpyrrolidine, m. 111°; heated with an excess EtOHKOH, it gives KCN, PhNH₂ and an oil from which I could be isolated. α-Benzoylethylmalonic acid (I), m. 164-5° (decomposition), was prepared in 1 step by condensing 20 g. PhCH(CN)NHPH and 18.6 g. MeCH:C(CO₂Et)₂ in 75 cc. EtOH with 50% aqueous KOH (2.2 g.) and after 2 hrs. adding 45.5 g. KOH and boiling 2 hrs.; 18.5 g. Et₂O-soluble oil was obtained, from which I crystallized. Heated at 160° I gives β-benzoylbutyric acid (II), m. 59-60°; semicarbazone, m. 177-8°. I was also synthesized from Ph α-bromoethyl ketone b.p. 110-2°, yellow oil with lachrymatory properties, and CHK(CO₂Et)₂ in C₆H₆. PhCH(CN)NMePh does not condense with MeCH:C(CO₂Et)₂; the action of alkali gives a yellow compound, m. 126-8°, which forms a HCl salt.

IT 861384-66-9P, 3-Pyrrolidinecarboxylic acid, 5-cyano-2-keto-4-methyl-1,5-diphenyl- 861582-70-9P, 3-Pyrrolidinecarboxylic acid, 5-cyano-2-keto-4-methyl-1,5-diphenyl-, ethyl ester

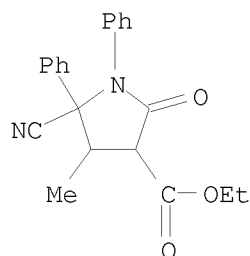
RL: PREP (Preparation)

(preparation of)

RN 861384-66-9 CAPLUS
 CN 3-Pyrrolidinecarboxylic acid, 5-cyano-4-methyl-2-oxo-1,5-diphenyl- (CA INDEX NAME)



RN 861582-70-9 CAPLUS
 CN 3-Pyrrolidinecarboxylic acid, 5-cyano-4-methyl-2-oxo-1,5-diphenyl-, ethyl ester (CA INDEX NAME)



L3 ANSWER 68 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1915:17111 CAPLUS
 DOCUMENT NUMBER: 9:17111
 ORIGINAL REFERENCE NO.: 9:2794i,2795a-d
 TITLE: Diketopyrrolidine derivatives.
 INVENTOR(S): Thiele, A.
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 1148637		19150803	US	

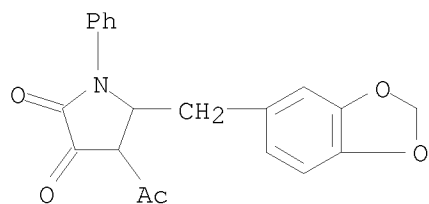
AB p-Methyl-diphenylbenzoyldiketopyrrolidine, crystalline m. 248° is made by heating p-toluidine with benzaldehyde in absolute alc., adding Et sodiobenzoylpyrrolidinate dissolved in absolute alc. and glacial HOAc, heating for 12 hrs. and precipitating with HCl, purifying through the Na salt and crystalline from alc. 1-o-Tolyl-2-phenyl-3-acetyl-4,5-diketopyrrolidine, rose colored crystalline, m. 177-9°, is made by reaction in Et₂O solution of o-toluidine and benzaldehyde on Et acetylpyrrolidinate. 1-o-Methoxyphenyl-2-phenyl-3-acetyl-4,5-diketopyrrolidine, m. 225-7° (decomposition), is made by reaction in ether solution of anisidine, benzaldehyde and Et acetylpyrrolidinate; 1-Phenyl-2-piperonyl-3-acetyl-4,5-diketopyrrolidine, m. 197°, by heating together aniline, piperonal and Et acetylpyrrolidinate, in C₆H₆. 1-p-Tolyl-2-p-dimethylaminophenyl-3-acetyl-4,5-diketopyrrolidine, a brown powder, m. 166° (decomposition), is made by reaction in C₆H₆ of Et acetylpyrrolidinate, p-toluidine and p-dimethylaminobenzaldehyde. 1-Quinolyl-2-phenyl-3-acetyl-4,5-diketopyrrolidine, m. 222° (decomposition), is made from

8-aminoquinoline, benzaldehyde and Et acetylpyrroacemate in C₆H₆ solution 1-[1-Phenyl-2,3-dimethyl-5-pyrazolyl]-2-phenyl-3-acetyl-4,5-diketopyrrolidine, a light brown powder, with a bitter taste, decompose on heating, is made from phenyldimethylaminopyrazolone, benzaldehyde and Et acetyl pyrroacemate, by heating in C₆H₆ at 100-10° for 5-6 hrs. 1-Phenyl-2-furfuryl-3-acetyl-4,5-diketopyrrolidine, yellow-green crystalline, soluble in alc. and ether and m. 190° (decomposition), is made by heating furfural, aniline and Et acetylpyrroacemate in C₆H₆ on a H₂O-bath for 2 hrs. 1-o-Methoxyphenyl-2-phenyl-3-benzoyl-4,5-diketopyrrolidine, crystalline m. 215-7° (decomposition), is made by reaction of o-anisidine, benzaldehyde and Et benzoylpyrroacemate in C₆H₆ for 24 hrs. All these compds. are insol. in H₂O, difficultly soluble in ether and C₆H₆, soluble in alkalis and stable when heated with dilute acids or alkalis. They are proposed for use as medicines.

IT 859958-02-4P, 4,5-Pyrroledione, 3-acetyl-2,3-dihydro-1-phenyl-2-piperonyl 860759-80-4P, 4,5-Pyrroledione, 3-acetyl-2-p-dimethylaminophenyl-2,3-dihydro-1-p-tolyl- 860759-81-5P, 4,5-Pyrroledione, 3-acetyl-2,3-dihydro-2-phenyl-1-o-tolyl-
RL: PREP (Preparation)
(preparation of)

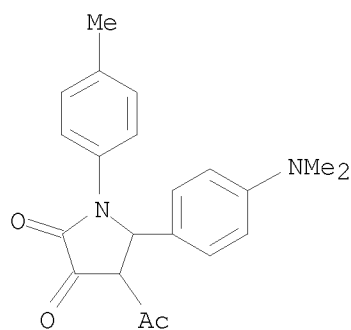
RN 859958-02-4 CAPLUS

CN 2,3-Pyrrolidinedione, 4-acetyl-5-(1,3-benzodioxol-5-ylmethyl)-1-phenyl-
(CA INDEX NAME)



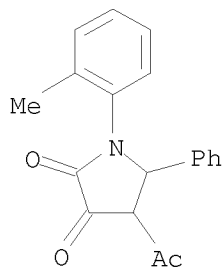
RN 860759-80-4 CAPLUS

CN 2,3-Pyrrolidinedione, 4-acetyl-5-[4-(dimethylamino)phenyl]-1-(4-methylphenyl)- (CA INDEX NAME)

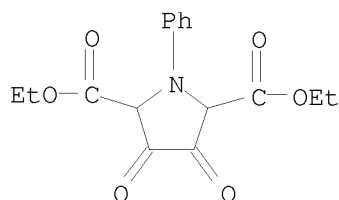


RN 860759-81-5 CAPLUS

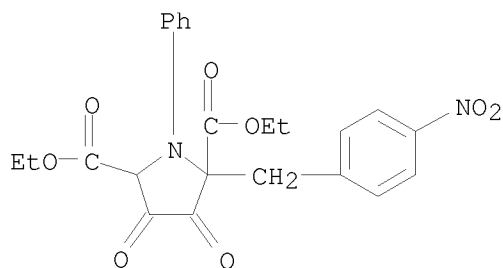
CN 2,3-Pyrrolidinedione, 4-acetyl-1-(2-methylphenyl)-5-phenyl- (CA INDEX NAME)



L3 ANSWER 69 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1911:15334 CAPLUS
 DOCUMENT NUMBER: 5:15334
 ORIGINAL REFERENCE NO.: 5:2642f-i
 TITLE: Synthesis of Pyrrole Compounds from Imido Acids.
 N-Phenyl- α,α' -Dicarbethoxy- β,β' -
 Diketopyrrolidine
 AUTHOR(S): Johnson, Treat B.; Bengis, Robert
 CORPORATE SOURCE: Sheffield Lab., Yale Univ.
 SOURCE: Journal of the American Chemical Society (1911), 33,
 745-55
 CODEN: JACSAT; ISSN: 0002-7863
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 GI For diagram(s), see printed CA Issue.
 AB In presence of EtONa, each of the 4 combinations of diethyl or dimethyl
 oxalate and diethyl or dimethyl N-phenyldiglycolamidate condense giving
 N-phenyl- α,α' -dicarbethoxy- β,β' -diketopyrrolidine,
 formula (I), needle-like prisms from hot alc. or AcOH, m. 137-8°.
 Similarly in MeONa the 4 combinations gave N-phenyl- α,α' -
 dicarbomethoxy- β,β' -diketopyrrolidine, crystals from hot alc. m.
 188-9°, and in some cases a trace of (I). Mouilpied (J. Chemical
 Society, 87, 435) under similar conditions obtained 6 products, these were
 probably mixtures of these 2 compds. The yellow disodium salt of (I) when
 digested in alc. with an excess of a halide of an aromatic base yields the
 colorless monosodium salt. Barium salt. H₂O yellow. On digesting the
 disodium salt of (I) with nitrobenzyl chloride, 2 products were obtained.
 (a) N-phenyl- α,α' -dicarbethoxy- α -p-nitrobenzyl-
 β,β' -diketopyrrolidine (II), orange colored powder from alc. +
 H₂O, m. 180-2°, (b) the part insol. in alc. + H₂O gave
 di-(p-nitrobenzyl)-N-phenyl- α,α' -dicarbethoxy- β,β' -
 diketopyrrolidine, yellow prisms from AcOH, m. 132°. HI or Al
 amalgam do not reduce (I).
 IT 859957-84-9, 2,5-Pyrrolidinedicarboxylic acid,
 3,4-diketo-1-phenyl-, diethyl ester
 (and derivs.)
 RN 859957-84-9 CAPLUS
 CN 2,5-Pyrrolidinedicarboxylic acid, 3,4-dioxo-1-phenyl-, 2,5-diethyl ester
 (CA INDEX NAME)



IT 860759-52-0P, 2,5-Pyrrolidinedicarboxylic acid,
3,4-diketo-2-(p-nitrobenzyl)-1-phenyl-, diethyl ester
RL: PREP (Preparation)
(preparation of)
RN 860759-52-0 CAPLUS
CN 2,5-Pyrrolidinedicarboxylic acid, 2-[(4-nitrophenyl)methyl]-3,4-dioxo-1-
phenyl-, 2,5-diethyl ester (CA INDEX NAME)

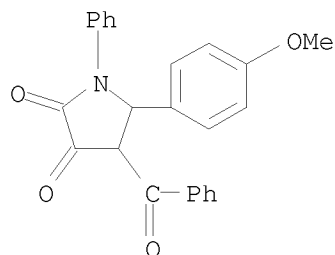


L3 ANSWER 70 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1910:1764 CAPLUS
DOCUMENT NUMBER: 4:1764
ORIGINAL REFERENCE NO.: 4:319h-i,320a-i,321a-h
TITLE: Syntheses of Cinchonic Acid
AUTHOR(S): Borsche, W.
CORPORATE SOURCE: Gen. Chem. Inst.;Univ. Gottingen
SOURCE: Berichte der Deutschen Chemischen Gesellschaft (1910),
42, 4072-88
CODEN: BDCGAS; ISSN: 0365-9496
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 4:1764
GI For diagram(s), see printed CA Issue.
AB α,β ,N-Triphenyl- α',β' -diketopyrrolidine, formula
(I)below, is prepared from phenylpyruvic acid, BzH and PhNH₂; colorless
needles, m. 250°. Yield, 80%. It is also formed from the acid and
benzalaniline. It does not react with ketone reagents. Acetate, crystalline
powder, m. 185°. Benzoate, crystalline, m. 174°. α,β ,N-Triphenyl- α' -keto- β' -hydroxypyrrolidine (II)
is produced from AcOH, Zn dust and (I); colorless crystals, m.
238°. Distillation decomposes it into stilbene, gases and a
compound C₂₁H₁₇ON; needles, m. about 338°. α,β -Diphenyl-
N-o-tolyl- α',β' -diketopyrrolidine (III) is prepared in a
similar manner to (I) by the use of o-toluidine; colorless, crystalline powder,
m. 232-4°. m-Tolyl derivative, brittle, yellow resin. p-Tolyl
compound, colorless crystals, m. 224°. α,β -Diphenyl-N-m-
nitrophenyl- α',β' -diketopyrrolidine (IV), from m-nitraniline;
pale yellow needles, m. 226°. β ,N-Diphenyl- α',β' -
diketopyrrolidine, from PhNH₂ and HCHO; crystalline powder, m. about
208°. β ,N-Diphenyl- α -p-nitrophenyl- α',β' -
diketopyrrolidine, from PhNH₂, and p-nitrobenzaldehyde; almost colorless
crystals, m. 192°. β ,N-Diphenyl- α ,o-hydroxyphenyl-
 α',β' -diketopyrrolidine, from PhNH₂ and salicylic aldehyde;
colorless needles, m. 252,°. β ,N-Diphenyl- β -p-
methoxyphenyl- α',β' -diketopyrrolidine, colorless crystals, m.
195°. When distilled it gives p-methoxystilbene.
 α,β -Diphenyl- β -naphthoquinoline- γ -carboxylic acid
(α,β -diphenyl- β -naphthocinchonic acid) (V) is prepared
from phenylpyruvic acid, BzH and β -naphthylamine; pale yellow, crystalline

powder, m. and evolves CO₂ about 275°. Yield, 40%. Sodium salt, hair-like needles. α,β -Diphenyl- β -naphthoquinoline (VI), formed by heating the acid; colorless needles from acetone or AcOH + H₂O, rhombic plates from AcOEt + alc., m. 179-80°. α -Methyl- β -phenyl- β -naphthocinchonic acid (VII), from phenylpyruvic acid, AcH and β -naphthylamine; colorless, highly insol. needles. When heated it gives β -phenyl- β -naphthoquinoline (VIII); yellow, pointed, acute-angled prisms with 1 H₂O, m. 101°. Hydrochloride and sulphate, colorless needles. Nitrate, lustrous plates. All the salts have a deep blue fluorescence in solution, it is specially intense in the case of the sulphate. β -Phenyl- β -naphthocinchonic acid (IX), from phenylpyruvic acid, HCHO and β -naphthylamine; colorless flocks. Yield, 22-5%. When heated it forms the quinoline derivative (X); needles with 2 H₂O, m. and evolves gas 111°. α,N -Diphenyl- β -o-nitrophenyl- α',β' -diketopyrrolidine (XI), from o-nitrophenylpyruvic acid, BzH and PhNH₂; yellowish plates, m. and decomposes 207-8°. Yield, 150% of the nitro acid. α -Phenyl- β -o-nitrophenyl- β -naphthocinchonic acid (XII), from o-nitrophenylpyruvic acid, BzH and β -naphthylamine; crystalline. Yield, 33%. When fused it gives α -phenyl- β -o-nitrophenyl- β -naphthoquinoline; yellow, rhombic plates which are stated to have 1 and also 0.5 mol. H₂O, m. 193-4°. o-Nitrophenylpyruvic acid, β -naphthylamine and HCHO also form a naphthocinchonic acid. Yield, about 22%. Benzoylpyruvic acid, BzH and PhNH₂ give α,N -diphenyl- β -benzoyl- α',β' -diketopyrrolidine (XIII); colorless needles, m. and darkens 242-4°. Anisic aldehyde forms the corresponding N-phenyl- α -p-methoxyphenyl- β -benzoyl- α',β' -diketopyrrolidine; colorless crystals, m. 228°. α -Phenyl- β -benzoyl- β -naphthocinchonic acid (XIV), from benzoylpyruvic acid, BzH and β -naphthylamine; colorless needles. Yield, 25%. When melted it gives the naphthoquinoline; colorless, slender, thickly felted needles, m. 185°. β -Benzoyl- β -naphthocinchonic acid (XV), from benzoylpyruvic acid, HCHO and β -naphthylamine; pale yellow, crystalline powder. Yield, 34%. When m. it passes into the corresponding quinoline; colorless needles, m. 108-9°. Benzylpyruvic acid, BzH and PhNH₂ form N, α -diphenyl- β -benzyl- α',β' -diketopyrrolidine (XVI); colorless needles, m. 196°. Yield, 100% of the acid. α -Phenyl- β -benzylcinchonic acid (XVII) is formed together with the preceding compound, from which it is separated by its solubility in aqueous Na₂CO₃; crystalline, m. 290°. Yield, 13%. When heated it gives α -phenyl- α -benzylquinoline; colorless needles, m. 96-7°. 2-Methyl- α -phenyl- β -benzylcinchonic acid (XVIII), from benzylpyruvic acid, BzH and m-toluidine; slender, colorless needles. Yield, about 35% of the acid. When fused it is converted into 2-methyl- α -phenyl- β -benzylquinoline; needles, m. 99°. Benzylpyruvic acid, BzH and β -naphthylamine form α -phenyl- β -benzyl- β -naphthocinchonic acid (XIX); pale yellow, crystalline powder. Yield, 57%. The corresponding naphthoquinoline is deposited in colorless needles, m. 152°. The following groups of quinoline- γ -carboxylic acids may be synthesized by means of Dobner's reaction. (1) α -Substituted γ -carboxylic acids from pyruvic acid, primary aromatic amines and homologues of HCHO. (2) β -Substituted (naphtho-) quinoline- γ -carboxylic acids, from monosubstituted pyruvic acid, HCHO and β -naphthylamine. (3) α,β -Disubstituted γ -carboxylic acids from monosubstituted pyruvic acid, primary aromatic amines and the homologues of HCHO (cf. following abstract).

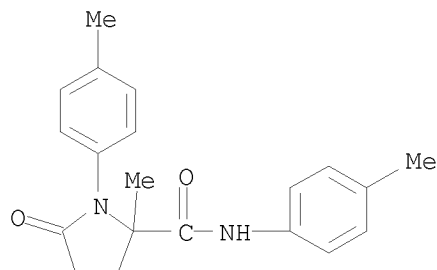
IT 859958-17-1P, 2,3-Pyrroledione, 5-p-anisyl-4-benzoyl-4,5-dihydro-1-phenyl-
 RL: PREP (Preparation)
 (preparation of)

RN 859958-17-1 CAPLUS
CN 2,3-Pyrrolidinedione, 4-benzoyl-5-(4-methoxyphenyl)-1-phenyl- (CA INDEX NAME)

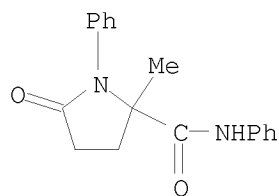


L3 ANSWER 71 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1909:14668 CAPLUS
DOCUMENT NUMBER: 3:14668
ORIGINAL REFERENCE NO.: 3:2696e-i,2697a-b
TITLE: Phthaleinoximes
AUTHOR(S): Meyer, Richard; Kissin, S. M.
CORPORATE SOURCE: Chem. Lab., Techn. Hochsch., Brunswick
SOURCE: Berichte der Deutschen Chemischen Gesellschaft (1909),
42, 2825-38
CODEN: BDCGAS; ISSN: 0365-9496
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB The constitution of the phthaleinoximes is discussed at considerable length; the results are expressed in the formulas given below. Benzoyl phenolphthaleinoxime, formula (I) below; colorless crystals, m. 175°. It is hydrolyzed with difficulty. The formula C₂₀H₁₅O₃N for the reduction product of phenolphthaleinoxime is confirmed. Hydroquinolphthalein- α -oxime trimethyl ether, by the action of Me₂SO₄; needles, m. 123-4°. Triacetyl derivative, crystalline, m. 210°. Tribenzoyl derivative, needles, m. 226-7°. The α -oxime (II) could not be reduced by means of Zn dust and NaOH, but the β -oxime (III), under these conditions, is converted into the γ -oxime (IV). γ -Oxime tribenzoyl derivative, yellow crystals, m. 275-80°, previously darkening. Hydroxyphenylphthalide oxime, colorless plates with 1 MeOH, m. 215-6°. Dibenzoyl derivative, colorless needles, m. 233-4°. Hydroxydiphenylphthalide oxime, colorless, cubical crystals from Et₂O, m. 204-5°, previously darkening. From alc. the crystals are yellow, but become colorless in Et₂O or when heated at 120°. Dibenzoyl derivative, colorless needles, m. 150-1°. Methylglutolactonic acid (V) does not yield an oxime, and it does not react with phenylhydrazine nor with bromophenylhydrazine (?); unsym. methylphenylhydrazine converts it into NH₄ methylglutolactonate. The following additional derivatives of this acid have been prepared. Dianilide, colorless needles, m. 205-6°. Di-p-toluide, colorless needles, m. 198-9°. The acid converts α - and β -naphthylamine into α - and β -dinaphthylamine respectively and it fails to react with the nitranilines and with m-toluylenediamine.
IT 859957-85-0P, 2-Pyrrolidinecarboxy-p-toluide, 5-keto-2-methyl-1-p-tolyl- 860759-04-2P, 2-Pyrrolidinecarboxanilide, 5-keto-2-methyl-1-phenyl-
RL: PREP (Preparation)
(preparation of)
RN 859957-85-0 CAPLUS

CN 2-Pyrrolidinecarboxamide, 2-methyl-N,1-bis(4-methylphenyl)-5-oxo- (CA INDEX NAME)



RN 860759-04-2 CAPLUS
CN 2-Pyrrolidinecarboxamide, 2-methyl-5-oxo-N,1-diphenyl- (CA INDEX NAME)



L3 ANSWER 72 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1909:10755 CAPLUS

DOCUMENT NUMBER: 3:10755

ORIGINAL REFERENCE NO.: 3:1992f-i,1993a

TITLE: Formation and Reactions of Imino Compounds. VIII. The formation of Methyl Derivatives of 2-Phenyl-1,3-Naphthalenediamine from the Three Tolylacetonitriles

AUTHOR(S): Best, S. R.; Thorpe, J. F.

SOURCE: Journal of the Chemical Society, Transactions (1909), 95, 261-73

CODEN: JCHTA3; ISSN: 0368-1645

DOCUMENT TYPE: Journal

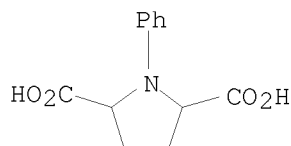
LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

AB By condensing o-tolylacetonitrile with 1 mol. Na, finely divided by melting and shaking in xylene and pouring off the solvent, and a trace of EtOH, β -imino- α -cyano- α,γ -di-o-tolylpropane, $\text{MeC}_6\text{H}_4\text{CH}_2\text{C}(\text{:NH})\text{CH}(\text{CN})\text{C}_6\text{H}_4\text{Me}$, is formed; viscous liquid, b13 270-80°. On washing the Et2O soluble of the above, after steam distillation, with dilute HCl, separating and treating with dilute Na_2CO_3 , 6-amino-5-o-tolyl-2,4-di-o-methylbenzylpyrimidine, is secured. It separates from alc. in colorless needles, m. 1.40-1°. If this product is more desired than the first described the condensation can be carried out in an alc. soluble of NaOEt when it is obtained by filtering the soluble before distilling with steam. By treating the β -imino- α -cyano- α,γ -di-o-tolylpropane with cold concentrate H_2SO_4 , 6-o-tolyl-1-methyl-5,7-naphthalenediamine is formed; colorless plates, m. 136°. Dihydrochloride and diacetyl derivative Similarly, 6-amino-5-m-tolyl-2.4-di-m-methylbenzylpyrimidine, m. 147°; small needles, and β -imino- α -cyano- α,γ -di-m-tolylpropane, b18 275-80° have been prepared. From the latter, by treatment with

H₂SO₄, 6-m-tolyl-2-methyl-5, 7-naphthylenediamine is made; small plates, m. 143°. This oxidizes by K₃Cr₂O₇ to 4-methylphthalic acid. Dihydrochloride and diacetyl derivative, also the pyrimidine hydrochloride. The corresponding p-pyrimidine; concentric needles, m. 117-20°. Hydrochloride, β-imino-α-cyano-α,γ-di-p-tolylpropane, b₁₈ 280-83°. With H₂SO₄ it yields 7-p-tolyl-2-methyl-6,8-naphthalenediamine; glistening plates, m. 160°. Dihydrochloride and diacetyl derivative. When the 3 β-imino-α cyano-α,γ-ditolylpropanes are treated with H₂SO₄ the binding influence of a Me group in the m-position on the formation of the naphthalene ring at a certain C atom is clearly seen. The yield from compounds where the Me-group is in the m-position is only 10% while with the other 80% is obtained.

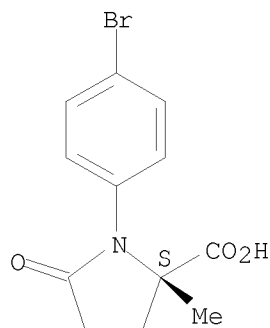
IT 859957-82-7, 2,5-Pyrrolidinedicarboxylic acid, 1-phenyl-
(and derivs., from adipic acid)
RN 859957-82-7 CAPLUS
CN 2,5-Pyrrolidinedicarboxylic acid, 1-phenyl- (CA INDEX NAME)



L3 ANSWER 73 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1908:988 CAPLUS
DOCUMENT NUMBER: 2:988
ORIGINAL REFERENCE NO.: 2:278e-i,279a
TITLE: Condensation Products of Ethyl Levulinate, Hydrogen Cyanide and p-Substituted Anilines
AUTHOR(S): Weber, Hermann
CORPORATE SOURCE: Techn. Inst.;Univ. Berlin
SOURCE: Berichte der Deutschen Chemischen Gesellschaft (1908), 40, 4044-52
CODEN: BDCGAS; ISSN: 0365-9496
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB Ethyl levulinate, hydrogen cyanide and p-chloraniline yield 1-p-chlorophenyl-2-methylpyrrolidone-carboxylic nitrile, crystalline, m. 40-2°. Amide, prismatic needles, m. 207°. Acids, colorless needles, m. 179°. Barium salt, broad prisms with 1H₂O. Methyl ester, crystalline. p-Bromaniline yields, similarly, the nitrile, slender, yellow needles, m. 49-51°. Amide, prismatic rods, m. 208°. Carboxylic acid, slender, colorless, interlaced needles, m. 189°. Silver salt, short prisms. Barium salt, short, prismatic needles with 1H₂O. Methyl ester, short prisms. The nitrile is converted by NH₄O.HCl into γ-hydroxyiminovaleric acid. The nitrile from p-iodoaniline is an oil. Amide, prismatic needles, m. 222°. Carboxylic acid, thin, colorless needles, m. 211-2°. Silver salt, short prisms, becoming brown on exposure to light. Methyl ester, brown, viscid oil. p-Aminobenzonitrile, treated in the same manner as the anilines, forms a crystalline compound, m. 77°. The yield is very small and no well defined derivatives could be prepared. Ethyl levulinate, hydrogen cyanide and ethyl p-aminobenzoate combine, forming the open chain derivative, EtO₂CC₆H₄NH₂Me(CN)CH₂CH₂CO₂Et; crystalline, m. 75°. It is converted by HCl into the carboxylic acid, prisms with 1H₂O m. 228-9°. Amide, crystalline, m. 149°. Amide from methyl p-aminobenzoate, crystalline, m. 171-2°.

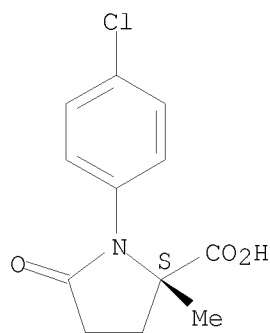
IT 904813-38-3, Proline, 1-(p-bromophenyl)-5-keto-2-methyl-
 908578-57-4, Proline, 1-(p-chlorophenyl)-5-keto-2-methyl-
 908578-68-7, Proline, 1-(p-iodophenyl)-5-keto-2-methyl-
 (and derivs.)
 RN 904813-38-3 CAPLUS
 CN Proline, 1-(p-bromophenyl)-5-keto-2-methyl- (1CI) (CA INDEX NAME)

Absolute stereochemistry.



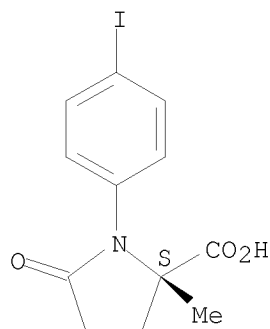
RN 908578-57-4 CAPLUS
 CN Proline, 1-(p-chlorophenyl)-5-keto-2-methyl- (1CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 908578-68-7 CAPLUS
 CN Proline, 1-(p-iodophenyl)-5-keto-2-methyl- (1CI) (CA INDEX NAME)

Absolute stereochemistry.

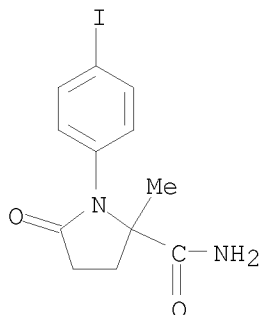


IT 859957-91-8P, 2-Pyrrolidinecarboxamide, 1-(p-iodophenyl)-5-keto-2-

methyl- 859957-93-0P, 2-Pyrrolidinecarboxamide,
 1-(p-chlorophenyl)-5-keto-2-methyl- 860759-08-6P,
 2-Pyrrolidinecarboxamide, 1-(p-carboxyphenyl)-5-keto-2-methyl-, methyl
 ester 860759-10-0P, 2-Pyrrolidinecarboxamide,
 1-(p-carboxyphenyl)-5-keto-2-methyl- 908578-59-6P, Proline,
 1-(p-carboxyphenyl)-5-keto-2-methyl-
 RL: PREP (Preparation)
 (preparation of)

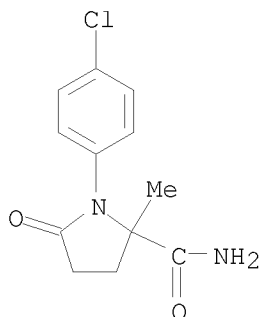
RN 859957-91-8 CAPLUS

CN 2-Pyrrolidinecarboxamide, 1-(4-iodophenyl)-2-methyl-5-oxo- (CA INDEX
 NAME)



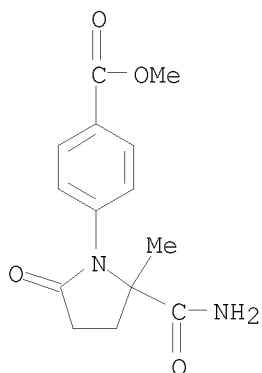
RN 859957-93-0 CAPLUS

CN 2-Pyrrolidinecarboxamide, 1-(4-chlorophenyl)-2-methyl-5-oxo- (CA INDEX
 NAME)

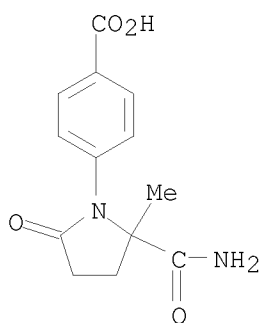


RN 860759-08-6 CAPLUS

CN Benzoic acid, 4-[2-(aminocarbonyl)-2-methyl-5-oxo-1-pyrrolidinyl]-, methyl
 ester (CA INDEX NAME)

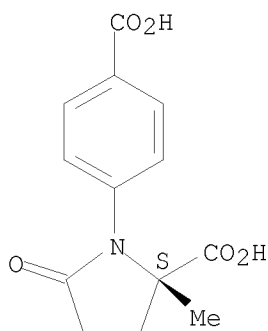


RN 860759-10-0 CAPLUS
 CN Benzoic acid, 4-[2-(aminocarbonyl)-2-methyl-5-oxo-1-pyrrolidinyl]- (CA INDEX NAME)



RN 908578-59-6 CAPLUS
 CN Proline, 1-(p-carboxyphenyl)-5-keto-2-methyl- (1CI) (CA INDEX NAME)

Absolute stereochemistry.



=>

=> FIL SINGUIDE
 COST IN U.S. DOLLARS
 FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
115.41	303.31

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-16.80	-16.80

FILE 'STNGUIDE' ENTERED AT 17:32:42 ON 24 APR 2008
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FILE CONTAINS CURRENT INFORMATION.
 LAST RELOADED: Apr 18, 2008 (20080418/UP).

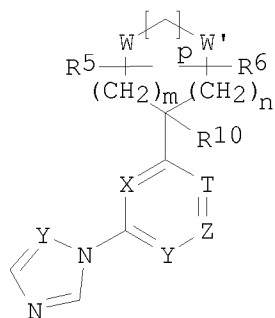
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 YOU HAVE REQUESTED DATA FROM FILE 'CAPLUS' - CONTINUE? (Y)/N:y

L3 ANSWER 32 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2006:510936 CAPLUS
 DOCUMENT NUMBER: 145:8185
 TITLE: Preparation of heterocyclic inhibitors of inducible
 nitric oxide synthase dimerization for therapeutic use
 INVENTOR(S): Gahman, Timothy C.; Lang, Hengyuan; Herbert, Mark R.;
 Thayer, Angelina M.; Hassig, Christian A.; Noble,
 Stewart A.; Cousins, Russell D.; Zhuang, Hui; Santos,
 Christopher R.; Chen, Xiaohong
 PATENT ASSIGNEE(S): Kalypsys, Inc., USA
 SOURCE: U.S. Pat. Appl. Publ., 108 pp.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

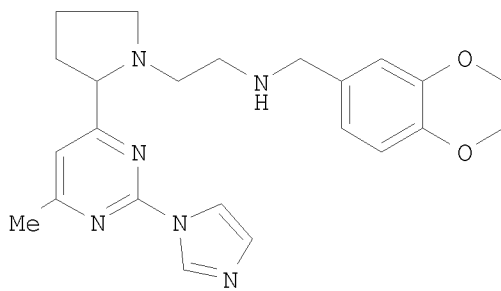
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20060116515	A1	20060601	US 2005-288888	20051128
AU 2005311985	A1	20060608	AU 2005-311985	20051128
CA 2589433	A1	20060608	CA 2005-2589433	20051128
WO 2006060424	A2	20060608	WO 2005-US43190	20051128
WO 2006060424	A3	20070329		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
EP 1817030	A2	20070815	EP 2005-852447	20051128
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, YU				
IN 2007KN01890	A	20070810	IN 2007-KN1890	20070525
KR 2007084574	A	20070824	KR 2007-711898	20070525
CN 101123962	A	20080213	CN 2005-80040524	20070525
PRIORITY APPLN. INFO.:		US 2004-631971P	P	20041201
		US 2005-672001P	P	20050414

OTHER SOURCE(S):
GI

MARPAT 145:8185



I



II

AB The present invention relates to compds. and methods useful as inhibitors of inducible nitric oxide synthase dimerization. Certain compds. of the subject invention have the following structural formula I: wherein T, V, X, and Y = CR₄ and N; Z = CR₃ and N; W and W' = CH₂, CR₇R₈, NR₉, O, NO, S(O)_q and CO; n, m and p = 0-5; q = 0-2; R₃, R₄, R₁₀ = H, halogen, optionally substituted alkyl, haloalkoxy, etc.; and R₇, R₈, and R₉ = H, halogen, optionally substituted alkyl, optionally substituted aralkyl, etc. Other compds. of the subject invention have structural formulas as defined in the invention. Also disclosed herein are pharmaceutical compns. comprising the compds. of the subject invention. The compds. of the invention can be used to inhibit or modulate NO synthesis and/or to lower NO levels in a patient. The preparation of the compds. is exemplified. For example, II was prepared from 2-[2-(2-imidazol-1-yl-6-methylpyrimidin-4-yl)pyrrolidin-1-yl]ethylamine and 2,3-dihydrobenzo[1,4]dioxin-6-carboxaldehyde. In HEK293 cells transiently transfected with human iNOS, II had an EC₅₀ of <1 μM.

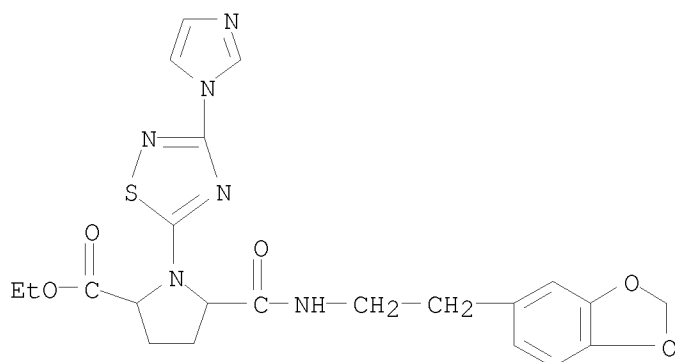
IT 888312-95-6P, 5-[[2-(Benzodioxol-5-yl)ethyl]carbamoyl]-1-[3-(imidazol-1-yl)-[1,2,4]thiadiazol-5-yl]pyrrolidine-2-carboxylic acid ethyl ester 888312-96-7P 888312-97-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

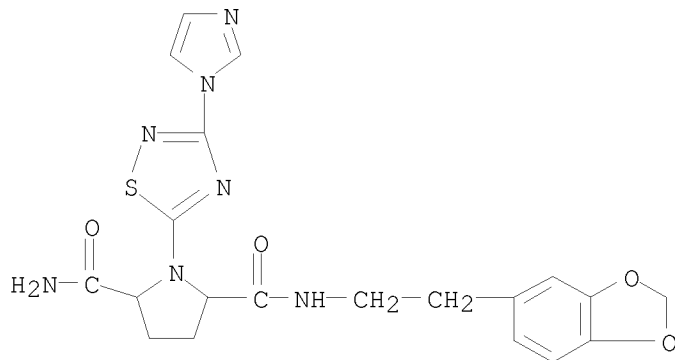
(drug candidate; preparation of heterocyclic inhibitors of inducible nitric oxide synthase dimerization for therapeutic use)

RN 888312-95-6 CAPLUS

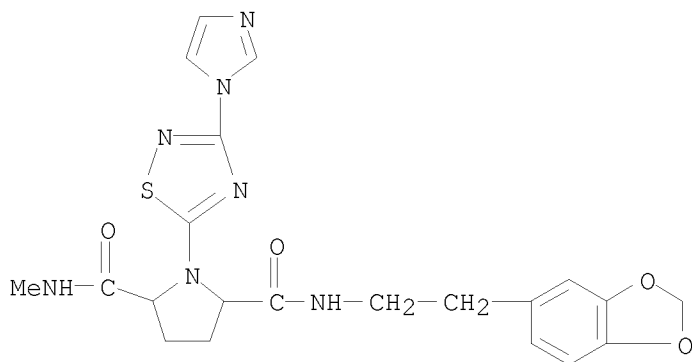
CN Proline, 5-[[[2-(1,3-benzodioxol-5-yl)ethyl]amino]carbonyl]-1-[3-(1H-imidazol-1-yl)-1,2,4-thiadiazol-5-yl]-, ethyl ester (CA INDEX NAME)



RN 888312-96-7 CAPLUS
 CN 2,5-Pyrrolidinedicarboxamide, N2-[2-(1,3-benzodioxol-5-yl)ethyl]-1-[3-(1H-imidazol-1-yl)-1,2,4-thiadiazol-5-yl]- (CA INDEX NAME)

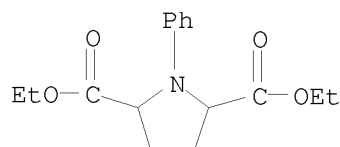


RN 888312-97-8 CAPLUS
 CN 2,5-Pyrrolidinedicarboxamide, N2-[2-(1,3-benzodioxol-5-yl)ethyl]-1-[3-(1H-imidazol-1-yl)-1,2,4-thiadiazol-5-yl]-N5-methyl- (CA INDEX NAME)

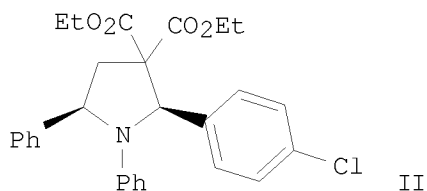
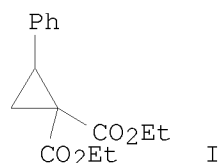


L3 ANSWER 33 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2006:359359 CAPLUS
 Correction of: 2005:1110275
 DOCUMENT NUMBER: 145:471313
 Correction of: 143:346991
 TITLE: Product class 10: γ -Lactams and larger ring lactams
 AUTHOR(S): Smith, M. B.
 CORPORATE SOURCE: Germany
 SOURCE: Science of Synthesis (2005), 21, 647-711
 CODEN: SSCYJ9
 PUBLISHER: Georg Thieme Verlag
 DOCUMENT TYPE: Journal; General Review
 LANGUAGE: English
 AB A review of the preparation of γ -lactams and larger ring lactams focusing on the use of acyclic and cyclic precursors.
 IT 910810-49-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of γ -lactams and larger ring lactams)
 RN 910810-49-0 CAPLUS

CN 2,5-Pyrrolidinedicarboxylic acid, 1-phenyl-, 2,5-diethyl ester (CA INDEX NAME)

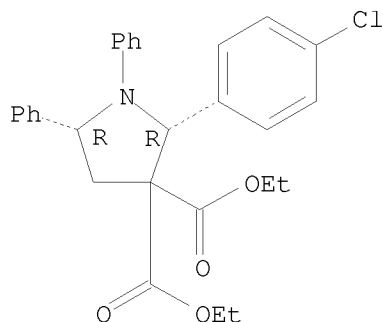


L3 ANSWER 34 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:15992 CAPLUS
DOCUMENT NUMBER: 144:253959
TITLE: Scandium triflate catalyzed cycloaddition of imines with 1,1-cyclopropanediester: efficient and diastereoselective synthesis of multisubstituted pyrrolidines
AUTHOR(S): Kang, Yan-Biao; Tang, Yong; Sun, Xiu-Li
CORPORATE SOURCE: State Key Laboratory of Organometallic Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai, 200032, Peop. Rep. China
SOURCE: Organic & Biomolecular Chemistry (2006), 4(2), 299-301
CODEN: OBCRAK; ISSN: 1477-0520
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:253959
GI



AB A tandem ring-opening-cyclization reaction of cyclopropanes with imines in the presence of 5 mol% of scandium triflate was developed for the highly diastereoselective synthesis of multisubstituted pyrrolidines. E.g., reaction of 1,1-cyclopropane diester I with PhN:CHC6H4Cl-4, catalyzed by scandium triflate, gave the cis isomer of pyrrolidine II.
IT 877035-09-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(diastereoselective synthesis of multisubstituted pyrrolidines by scandium triflate catalyzed cycloaddn. of imines with 1,1-cyclopropane diesters)
RN 877035-09-1 CAPLUS
CN 3,3-Pyrrolidinedicarboxylic acid, 2-(4-chlorophenyl)-1,5-diphenyl-, 3,3-diethyl ester, (2R,5R)-rel- (CA INDEX NAME)

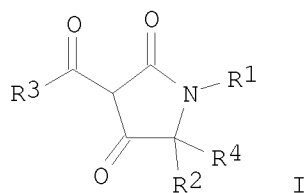
Relative stereochemistry.



REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 35 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2006:2507 CAPLUS
 DOCUMENT NUMBER: 144:412355
 TITLE: Method of preparation 3-acylpyrrolidine-2,4-dione compounds as herbicides
 INVENTOR(S): Yang, Huazheng; Zhu, Youquan; Zou, Xiaomao; Hu, Fangzhong; Liu, Bin; Yang, Xiufeng
 PATENT ASSIGNEE(S): Nankai University, Peop. Rep. China
 SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 22 pp.
 CODEN: CNXXEV
 DOCUMENT TYPE: Patent
 LANGUAGE: Chinese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1676515	A	20051005	CN 2005-10013206	20050317
PRIORITY APPLN. INFO.:			CN 2005-10013206	20050317
OTHER SOURCE(S):			CASREACT 144:412355; MARPAT 144:412355	
GI				



AB 3-Acylpyrrolidine-2,4-dione compds. I [R1= H, alkyl, alkoxyalkyl, haloalkyl, haloalkoxyalkyl, alkoxycarbonyl, alkenyl, haloalkenyl, substituted Ph, phenylalkyl; R2, R4= H, alkyl, alkoxy, phenylalkoxy, hydroxyalkyl, alkoxyalkyl, alkoxycarbonyl, haloalkyl, cyano; R3= H, alkyl, alkoxyalkyl, substituted heterocyclic, heterocyclic Ph, heterocyclic alkyl, heterocyclic alkoxy, heterocyclic alkylphenyl, Ph, phenoxyphenyl, phenylalkyl, aryl] useful as herbicides is prepared by treating substituted benzoyl ethyl acetate with Et N-substituted glycinate (at mole ratio of 1:1.5-3.0) at 60-100°C for 10-48 h, cooling to room temperature, adding sodium methoxide solution, and reacting at room temperature for 20-60 h.

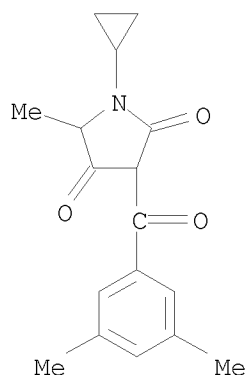
IT 884493-97-4P
 RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN

(Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of acylpyrrolidine dione derivative as herbicides)

RN 884493-97-4 CAPLUS

CN 2,4-Pyrrolidinedione, 1-cyclopropyl-3-(3,5-dimethylbenzoyl)-5-methyl- (CA INDEX NAME)



L3 ANSWER 36 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:1300785 CAPLUS

DOCUMENT NUMBER: 145:27790

TITLE: Synthesis, properties, and antimicrobial activity of 3-hydrazones of 1-aryl-5-methyl-1,5-ethoxycarbonylpyrrolidine-2,3-diones

AUTHOR(S): Gein, V. L.; Gein, L. F.; Chirkova, M. V.; Mikhalev, V. A.; Voronina, E. V.

CORPORATE SOURCE: Perm State Pharmaceutical Academy, Perm, Russia

SOURCE: Pharmaceutical Chemistry Journal (2005), 39(8), 413-417

CODEN: PCJOAU; ISSN: 0091-150X

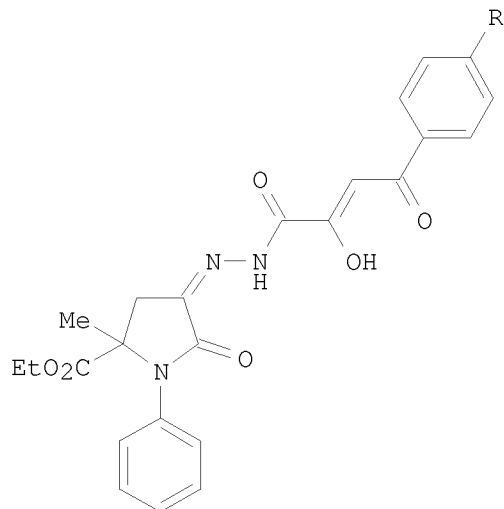
PUBLISHER: Springer

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 145:27790

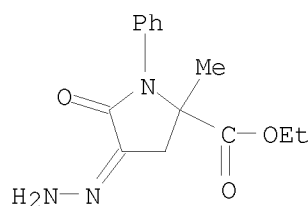
GI



AB Reactions of 5-methyl-1-aryl-ethoxycarbonylpyrrolidine-2,3-diones with hydrazine hydrate, phenylhydrazine, isoniazid, benzoylhydrazine, and thiosemicarbazide were used to synthesize a series of corresponding 3-hydrazones. All target products were obtained with a yield of 51 - 90%. The reactions of 3-hydrazone of 1-phenyl-5-methyl-5-ethoxycarbonylpyrrolidine-2,3-dione with 5-aryl-2,3-dihydro-2,3-furandiones yielded 3-N-arylpyruvoylhydrazones of 5-methyl-1-phenyl-5-ethoxycarbonylpyrrolidine-2,3-dione I (R = H or Me). The condensation of 3-hydrazone of 5-methyl-1-(4-chlorophenyl)-5-ethoxycarbonylpyrrolidine-2,3-dione with 4-methoxybenzaldehyde led to the 5-methyl-3-N-4-methoxybenzylidene-hydrazino-1-(4-chlorophenyl)-5-ethoxycarbonyl-3-pyrrolidin-2-one. The synthesized compds. were characterized by physicochem. consts. and the parameters of IR and ¹H NMR spectra. Some compds. were tested for antimicrobial activity.

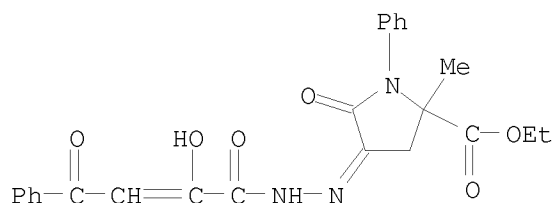
IT 889101-11-5P
 RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and antimicrobial activity of aroyl(pyruvoyl)hydrazones of (phenyl)ethoxycarbonyl(pyrrolidine)dione via its condensation with hydrazine followed by condensation with aryl(dihydro)furandiones)

RN 889101-11-5 CAPLUS
 CN Proline, 4-hydrazono-2-methyl-5-oxo-1-phenyl-, ethyl ester (9CI) (CA INDEX NAME)

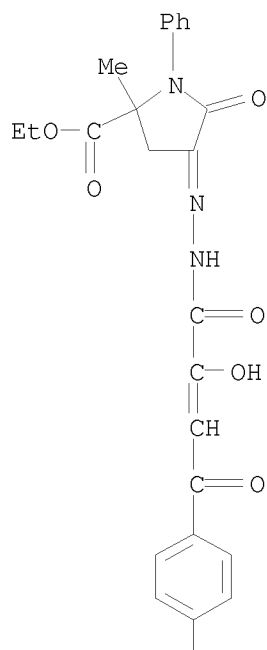


IT 889101-23-9P 889101-24-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and antimicrobial activity of aroyl(pyruvoyl)hydrazones of (phenyl)ethoxycarbonyl(pyrrolidine)dione via its condensation with hydrazine followed by condensation with aryl(dihydro)furandiones)

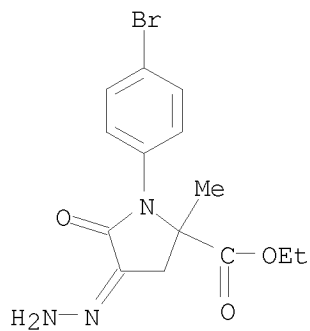
RN 889101-23-9 CAPLUS
 CN Proline, 4-[(2-hydroxy-1,4-dioxo-4-phenyl-2-butenyl)hydrazono]-2-methyl-5-oxo-1-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



RN 889101-24-0 CAPLUS
 CN Proline, 4-[[2-hydroxy-4-(4-methylphenyl)-1,4-dioxo-2-butenyl]hydrazono]-2-methyl-5-oxo-1-phenyl-, ethyl ester (9CI) (CA INDEX NAME)

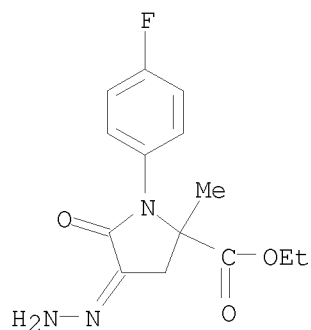


IT 889101-13-7P 889101-14-8P 889101-15-9P
 889101-19-3P 889101-22-8P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL
 (Biological study); PREP (Preparation)
 (preparation and antimicrobial activity of hydrazones of
 (aryl)ethoxycarbonyl(pyrrolidine)diones via their condensation with
 substituted hydrazines)
 RN 889101-13-7 CAPLUS
 CN Proline, 1-(4-bromophenyl)-4-hydrazono-2-methyl-5-oxo-, ethyl ester (9CI)
 (CA INDEX NAME)



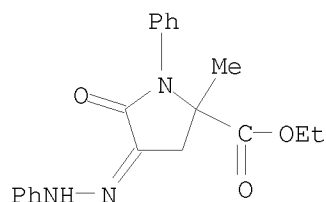
RN 889101-14-8 CAPLUS

CN Proline, 1-(4-fluorophenyl)-4-hydrazono-2-methyl-5-oxo-, ethyl ester (9CI)
(CA INDEX NAME)



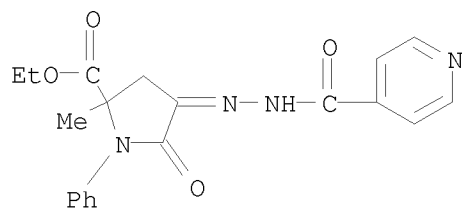
RN 889101-15-9 CAPLUS

CN Proline, 2-methyl-5-oxo-1-phenyl-4-(phenylhydrazono)-, ethyl ester (9CI)
(CA INDEX NAME)



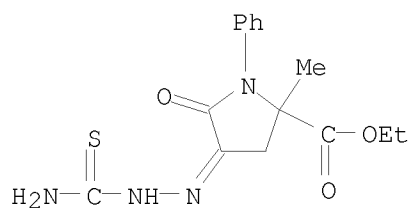
RN 889101-19-3 CAPLUS

CN 4-Pyridinecarboxylic acid, 2-[5-(ethoxycarbonyl)-5-methyl-2-oxo-1-phenyl-3-pyrrolidinylidene]hydrazide (CA INDEX NAME)



RN 889101-22-8 CAPLUS

CN Proline, 4-[(aminothioxomethyl)hydrazono]-2-methyl-5-oxo-1-phenyl-, ethyl ester (9CI) (CA INDEX NAME)

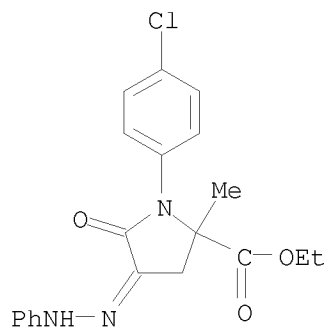


IT 889101-16-0P 889101-17-1P 889101-18-2P
889101-20-6P 889101-21-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and antimicrobial activity of hydrazones of
(aryl)ethoxycarbonyl(pyrrolidine)diones via their condensation with
substituted hydrazines)

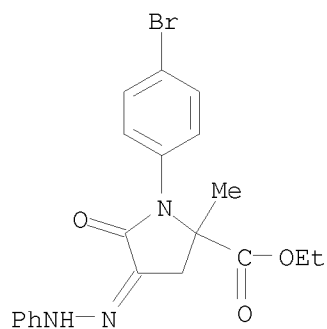
RN 889101-16-0 CAPLUS

CN Proline, 1-(4-chlorophenyl)-2-methyl-5-oxo-4-(phenylhydrazono)-, ethyl
ester (9CI) (CA INDEX NAME)



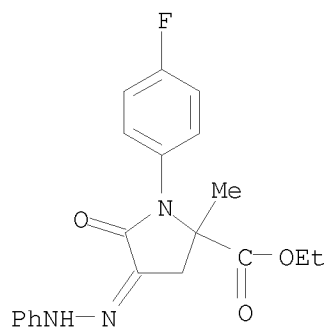
RN 889101-17-1 CAPLUS

CN Proline, 1-(4-bromophenyl)-2-methyl-5-oxo-4-(phenylhydrazono)-, ethyl
ester (9CI) (CA INDEX NAME)



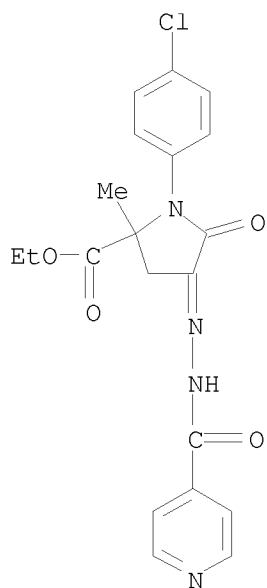
RN 889101-18-2 CAPLUS

CN Proline, 1-(4-fluorophenyl)-2-methyl-5-oxo-4-(phenylhydrazono)-, ethyl
ester (9CI) (CA INDEX NAME)



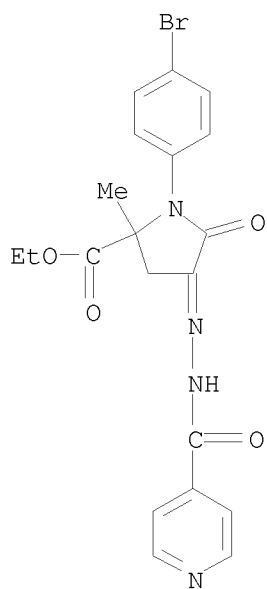
RN 889101-20-6 CAPLUS

CN 4-Pyridinecarboxylic acid, 2-[1-(4-chlorophenyl)-5-(ethoxycarbonyl)-5-
methyl-2-oxo-3-pyrrolidinylidene]hydrazide (CA INDEX NAME)



RN 889101-21-7 CAPLUS

CN 4-Pyridinecarboxylic acid, 2-[1-(4-bromophenyl)-5-(ethoxycarbonyl)-5-methyl-2-oxo-3-pyrrolidinylidene]hydrazide (CA INDEX NAME)



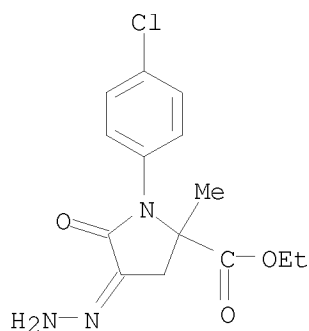
IT 889101-12-6P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(preparation and antimicrobial activity of methoxy(benzylidene)hydrazone of (chlorophenyl)ethoxycarbonyl(pyrrolidine)dione via its condensation with hydrazine followed by condensation with (methoxy)benzaldehyde)

RN 889101-12-6 CAPLUS

CN Proline, 1-(4-chlorophenyl)-4-hydrazono-2-methyl-5-oxo-, ethyl ester (9CI) (CA INDEX NAME)



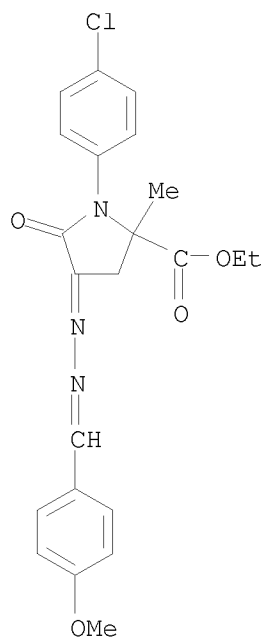
IT 889101-25-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and antimicrobial activity of methoxy(benzylidene)hydrazone of (chlorophenyl)ethoxycarbonyl(pyrrolidine)dione via its condensation with hydrazine followed by condensation with (methoxy)benzaldehyde)

RN 889101-25-1 CAPLUS

CN Proline, 1-(4-chlorophenyl)-4-[[4-methoxyphenyl)methylene]hydrazono]-2-methyl-5-oxo-, ethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT:

5

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 37 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:1269350 CAPLUS

DOCUMENT NUMBER: 145:8053

TITLE: Intramolecular 1,3-dipolar cycloaddition of azomethine ylides generated from ethoxycarbonyl carbenoids and Schiff bases

AUTHOR(S): Khlebnikov, A. F.; Novikov, M. S.; Kostikov, R. R.; Kopf, J.

CORPORATE SOURCE: St. Petersburg State University, St. Petersburg,
198504, Russia

SOURCE: Russian Journal of Organic Chemistry (2005), 41(9),
1341-1348
CODEN: RJOCEQ; ISSN: 1070-4280

PUBLISHER: Pleiades Publishing, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 145:8053

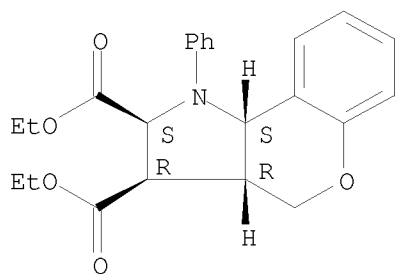
AB Decomposition of Et diazoacetate in the presence of copper, copper
acetylacetonate, or copper trifluoroacetylacetonate and Et
4-(2-iminophenoxyethyl)-2-butenates leads to formation of
chromeno[4,3-b]pyrrole-2,3-dicarboxylic acid derivs. The reactions
involve intermediate formation of azomethine ylides which undergo regio-
and stereoselective intramol. cycloaddn. at the C:C bond to afford
chromeno[4,3-b]pyrroles. The steric structure of the product depends on
the configuration of intermediate ylide and nature of the substituent at
the ylide nitrogen atom.

IT 887764-58-1P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(mol. structure; preparation of chromenopyrroles by stereoselective
intramol. 1,3-dipolar cycloaddn. of azomethine ylides from
ethoxycarbonyl carbenoids and Schiff bases)

RN 887764-58-1 CAPLUS

CN [1]Benzopyrano[4,3-b]pyrrole-2,3-dicarboxylic acid, 1,2,3,3a,4,9b-
hexahydro-1-phenyl-, 2,3-diethyl ester, (2R,3S,3aS,9bR)-rel- (CA INDEX
NAME)

Relative stereochemistry.



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 38 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:1163314 CAPLUS

DOCUMENT NUMBER: 144:88103

TITLE: Asymmetric Synthesis of Multifunctionalized Pyrrolines
by a Ruthenium Porphyrin-Catalyzed Three-Component
Coupling Reaction

AUTHOR(S): Xu, Hai-Wei; Li, Gong-Yong; Wong, Man-Kin; Che,
Chi-Ming

CORPORATE SOURCE: Shanghai-Hong Kong Joint Laboratory in Chemical
Synthesis, Shanghai Institute of Organic Chemistry,
The Chinese Academy of Science, Shanghai, 200032,
Peop. Rep. China

SOURCE: Organic Letters (2005), 7(24), 5349-5352
CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:88103

AB Chiral multifunctionalized pyrrolines have been synthesized by a ruthenium porphyrin catalyzed three-component coupling reaction. In a one-pot reaction, ruthenium porphyrins catalyzed in situ generation of chiral azomethine ylides from chiral diazo esters and imines. Asym. 1,3-dipolar cycloaddn. reactions of the chiral azomethine ylides with dipolarophiles afforded the pyrrolines in good yields and high diastereoselectivity (up to 92% de).

IT 871947-09-0P 872321-71-6P 872321-72-7P

872321-73-8P 872321-74-9P 872321-75-0P

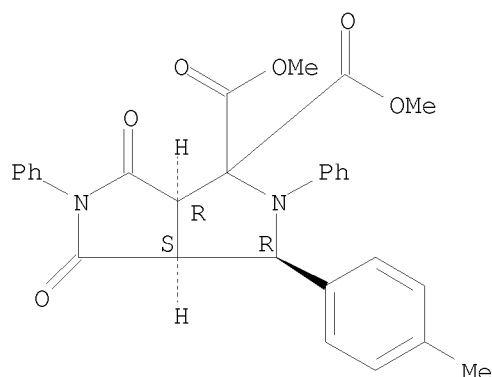
RL: SPN (Synthetic preparation); PREP (Preparation)

(asym. synthesis of multifunctionalized pyrrolines by a ruthenium porphyrin-catalyzed three-component coupling reaction)

RN 871947-09-0 CAPLUS

CN Pyrrolo[3,4-c]pyrrole-1,1(2H)-dicarboxylic acid, hexahydro-3-(4-methylphenyl)-4,6-dioxo-2,5-diphenyl-, 1,1-dimethyl ester, (3R,3aS,6aR)-rel- (CA INDEX NAME)

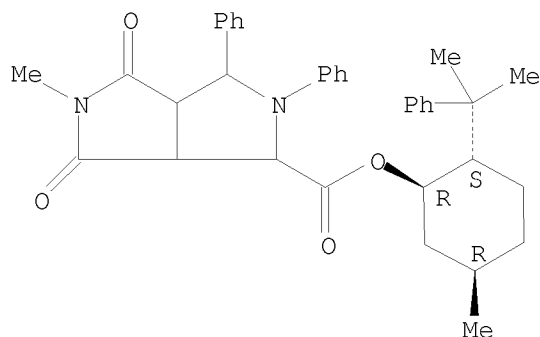
Relative stereochemistry.



RN 872321-71-6 CAPLUS

CN Pyrrolo[3,4-c]pyrrole-1-carboxylic acid, octahydro-5-methyl-4,6-dioxo-2,3-diphenyl-, (1R,2S,5R)-5-methyl-2-(1-methyl-1-phenylethyl)cyclohexyl ester (CA INDEX NAME)

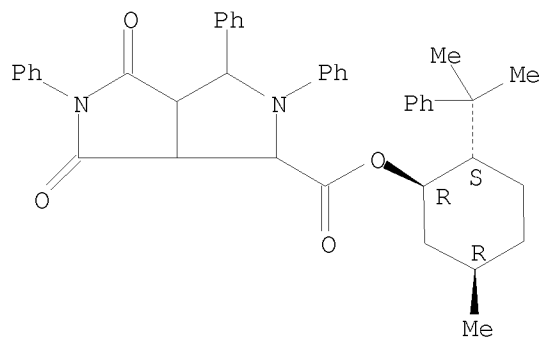
Absolute stereochemistry.



RN 872321-72-7 CAPLUS

CN Pyrrolo[3,4-c]pyrrole-1-carboxylic acid, octahydro-4,6-dioxo-2,3,5-triphenyl-, (1R,2S,5R)-5-methyl-2-(1-methyl-1-phenylethyl)cyclohexyl ester (CA INDEX NAME)

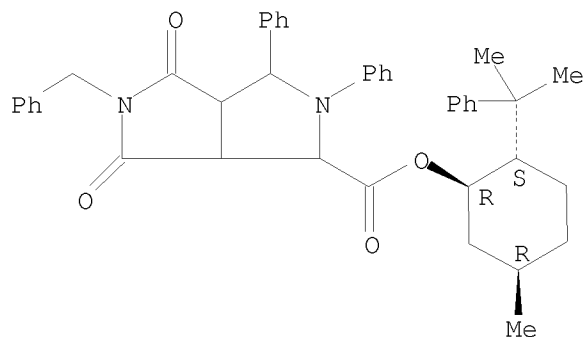
Absolute stereochemistry.



RN 872321-73-8 CAPLUS

CN Pyrrolo[3,4-c]pyrrole-1-carboxylic acid, octahydro-4,6-dioxo-2,3-diphenyl-5-(phenylmethyl)-, (1R,2S,5R)-5-methyl-2-(1-methyl-1-phenylethyl)cyclohexyl ester (CA INDEX NAME)

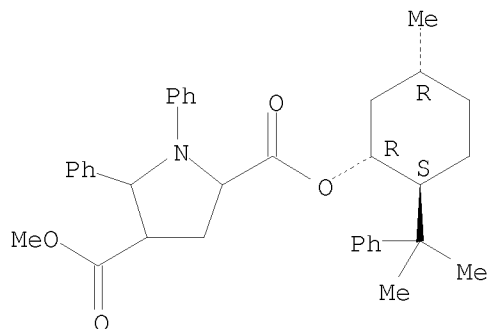
Absolute stereochemistry.



RN 872321-74-9 CAPLUS

CN 2,4-Pyrrolidinedicarboxylic acid, 1,5-diphenyl-, 4-methyl-2-[(1R,2S,5R)-5-methyl-2-(1-methyl-1-phenylethyl)cyclohexyl] ester (CA INDEX NAME)

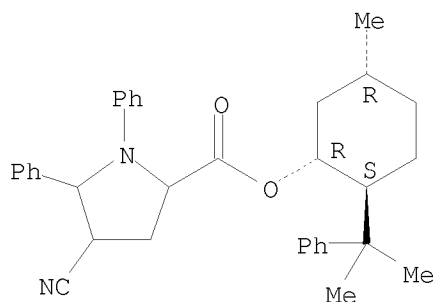
Absolute stereochemistry.



RN 872321-75-0 CAPLUS

CN Proline, 4-cyano-1,5-diphenyl-, (1R,2S,5R)-5-methyl-2-(1-methyl-1-phenylethyl)cyclohexyl ester (9CI) (CA INDEX NAME)

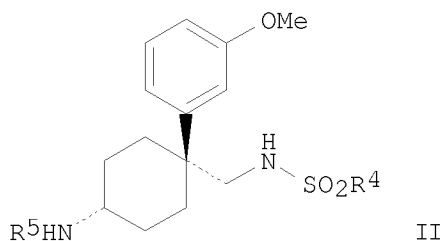
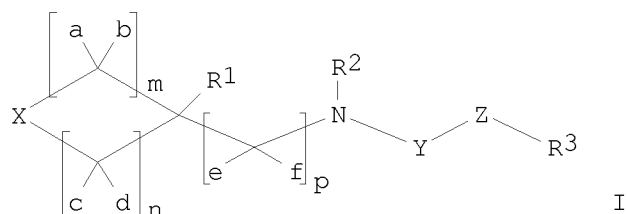
Absolute stereochemistry.



REFERENCE COUNT: 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

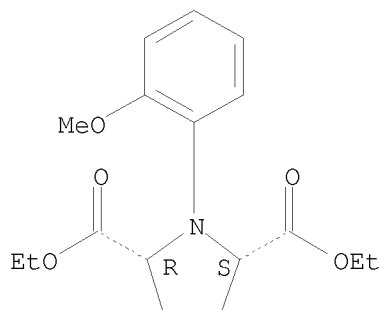
L3 ANSWER 39 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2005:1123880 CAPLUS
 DOCUMENT NUMBER: 143:405923
 TITLE: Preparation of heterocycle- and benzene-containing sulfonamide derivatives as LDL receptor agonists
 INVENTOR(S): Ban, Hitoshi; Asano, Shigehiro
 PATENT ASSIGNEE(S): Sumitomo Pharmaceuticals Co., Ltd., Japan
 SOURCE: PCT Int. Appl., 233 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005097738	A1	20051020	WO 2005-JP6977	20050404
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1736467	A1	20061227	EP 2005-728832	20050404
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				
PRIORITY APPLN. INFO.:			JP 2004-112503	A 20040406
			WO 2005-JP6977	W 20050404
OTHER SOURCE(S):			MARPAT 143:405923	
GI				



- AB Enhancers for expression of low d. lipoprotein receptor containing the title compds. represented by the formula (I), prodrugs thereof, and their pharmaceutically acceptable salts [m, n, p = 0-4 and 3≤m+n≤8; X = O, S, each (un)substituted NH or CH₂; R₁-R₃ = H, each (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heteroaryl, arylcarbonyl, heteroarylcarbonyl, arylsulfonyl, heteroarylsulfonyl, arylalkyl, or heteroarylalkyl; Y = SO₂, optionally esterified P(O)(OH), CO; Z = O, S, (un)substituted NH, (CH₂)_q; q = 0-4; a, b, c, d, e, f = H, HO, each (un)substituted alkyl, alkoxy, alkoxycarbonyl, aryl, heteroaryl, arylcarbonyl, heteroarylcarbonyl, arylalkyl, heteroarylalkyl, arylalkyloxy, or heteroarylalkyloxy; or one or plural combination(s) of a and b, c and d, or e and f represent oxo; e and f represent thioxo; a and c represent alkylene] are disclosed. Drugs for treating hyperlipemia and arteriosclerosis containing the compds. I are also disclosed. Thus, a solution of 40 mg tert-Bu [[[2-[cis-4-amino-1-(3-methoxyphenyl)cyclohexyl]methyl]amino]sulfonyl]carbamate and 22.0 mg 1-benzyl-4-piperidone in 2 mL 1,2-dichloroethane was treated with 71.7 mg sodium triacetoxyborohydride and stirred overnight, followed by treatment of the product with CF₃CO₂H in CH₂Cl₂ to give N-[[[cis-4-[(1-benzylpiperidin-4-yl)amino]-1-(3-methoxyphenyl)cyclohexyl]methyl]sulfonyl]carbamate (II) (R₄ = NH₂, R₅ = 1-benzyl-4-piperidinyl) (III). III and II (R₄ = Me, R₅ = 1,1'-biphenyl-4-ylmethyl) at 10 μM increased the uptake of 1,1'-dioctadecyl-3,3,3',3'-tetramethylindocarbocyanine perchlorate (DiI)-labeled human low d. lipoprotein in HepG2 cells by 230 and 238%, resp.
- IT 850887-29-5P, Diethyl cis-1-(2-methoxyphenyl)pyrrolidine-2,5-dicarboxylate
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of heterocycle- and benzene-containing sulfonamide derivs. as
- LDL receptor agonists for treatment of hyperlipemia and arteriosclerosis)
- RN 850887-29-5 CAPLUS
- CN 2,5-Pyrrolidinedicarboxylic acid, 1-(2-methoxyphenyl)-, 2,5-diethyl ester, (2S,5R)-rel- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 40 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:963979 CAPLUS

DOCUMENT NUMBER: 143:422221

TITLE: NaBH₄-InCl₃-Mediated One-Pot Chemo- and Stereoselective Decarboxylative Reduction of α -Aza gem-Dicarboxylic Esters to Monoalcohols

AUTHOR(S): Halder, Pranab; Ray, Jayanta K.

CORPORATE SOURCE: Department of Chemistry, Indian Institute of Technology, Kharagpur, 721302, India

SOURCE: Organic Letters (2005), 7(20), 4341-4343

CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 143:422221

AB The combination of NaBH₄ and a catalytic amount of InCl₃ provides a one-pot method for chemo- and stereoselective decarboxylative reduction of gem-dicarboxylic esters to monoalcs. in the presence of the lactam carbonyl in refluxing acetonitrile under inert atmospheric

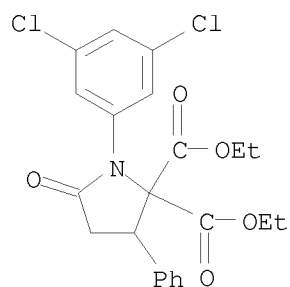
IT 868389-79-1 868389-80-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(NaBH₄-InCl₃-mediated one-pot chemo- and stereoselective decarboxylative reduction of oxopyrrolidinedicarboxylates to oxopyrrolidinemethanols)

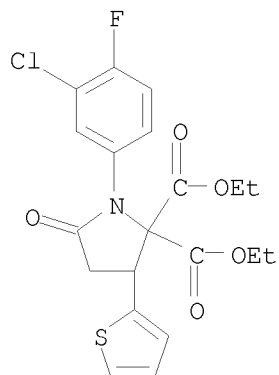
RN 868389-79-1 CAPLUS

CN 2,2-Pyrrolidinedicarboxylic acid, 1-(3,5-dichlorophenyl)-5-oxo-3-phenyl-, 2,2-diethyl ester (CA INDEX NAME)



RN 868389-80-4 CAPLUS

CN 2,2-Pyrrolidinedicarboxylic acid, 1-(3-chloro-4-fluorophenyl)-5-oxo-3-(2-thienyl)-, 2,2-diethyl ester (CA INDEX NAME)



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 41 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:943557 CAPLUS

DOCUMENT NUMBER: 144:292438

TITLE: Diastereoselective allylation of imines with γ -silyloxyallylstannanes promoted by trimethylsilyl triflate and application to the synthesis of erythro-sphingosine

AUTHOR(S): Shimizu, Makoto; Ando, Hiromi; Niwa, Yasuki

CORPORATE SOURCE: Department of Chemistry for Materials, Mie University, Mie, 514-8507, Japan

SOURCE: Letters in Organic Chemistry (2005), 2(6), 512-514

CODEN: LOCEC7; ISSN: 1570-1786

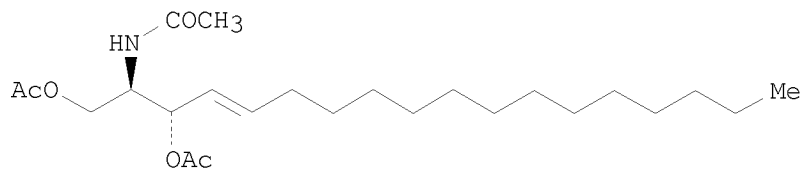
PUBLISHER: Bentham Science Publishers Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:292438

GI



I

AB Addition of γ -silyloxyallylstannanes to imines in the presence of trimethylsilyl triflate was studied. Allylation of α -imino ester with (Z)-allylstannane proceeded to give anti-adduct as a major product, which was transformed into N,O,O-triacetyl erythro-sphingosine (I) via appropriate functional group transformations.

IT 879215-07-3P 879215-08-4P 879215-09-5P

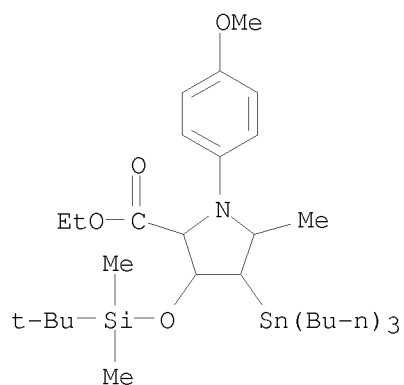
879215-10-8P 879215-11-9P

RL: BYP (Byproduct); PREP (Preparation)

(diastereoselective allylation of imines with γ -silyloxyallylstannanes promoted by trimethylsilyl triflate and application to the synthesis of erythro-sphingosine)

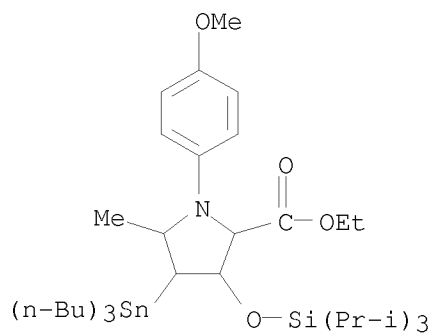
RN 879215-07-3 CAPLUS

CN Proline, 3-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1-(4-methoxyphenyl)-5-methyl-4-(tributylstannyl)-, ethyl ester (CA INDEX NAME)



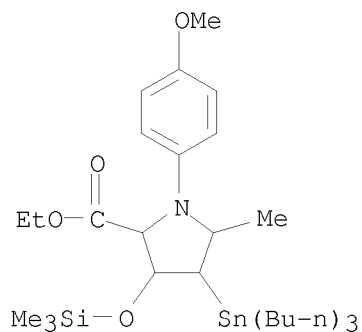
RN 879215-08-4 CAPLUS

CN Proline, 1-(4-methoxyphenyl)-5-methyl-4-(tributylstannyl)-3-[[tris(1-methylethyl)silyl]oxy]-, ethyl ester (CA INDEX NAME)



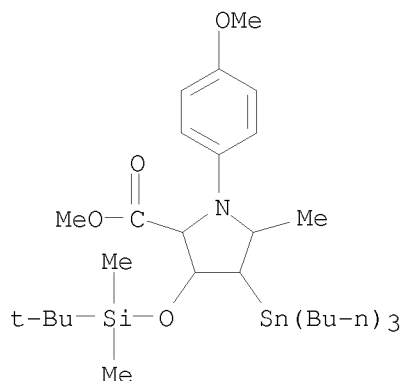
RN 879215-09-5 CAPLUS

CN Proline, 1-(4-methoxyphenyl)-5-methyl-4-(tributylstannyl)-3-[(trimethylsilyl)oxy]-, ethyl ester (CA INDEX NAME)



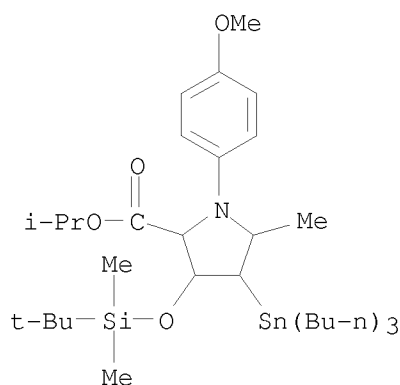
RN 879215-10-8 CAPLUS

CN Proline, 3-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1-(4-methoxyphenyl)-5-methyl-4-(tributylstannyl)-, methyl ester (CA INDEX NAME)



RN 879215-11-9 CAPLUS

CN Proline, 3-[[[1,1-dimethylethyl]dimethylsilyl]oxy]-1-(4-methoxyphenyl)-5-methyl-4-(tributylstannyl)-, 1-methylethyl ester (CA INDEX NAME)



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 42 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:921231 CAPLUS

DOCUMENT NUMBER: 143:367177

TITLE: Diastereoselective Synthesis of Pyrrolidines via the Yb(OTf)₃ Catalyzed Three-Component Reaction of Aldehydes, Amines, and 1,1-Cyclopropanediester

AUTHOR(S): Carson, Cheryl A.; Kerr, Michael A.

CORPORATE SOURCE: Department of Chemistry, University of Western Ontario, London, ON, N6A 5B7, Can.

SOURCE: Journal of Organic Chemistry (2005), 70(20), 8242-8244 CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 143:367177

AB Aldimines, generated in situ by the reaction of primary amines or anilines with aldehydes, undergo smooth reaction with various 1,1-cyclopropanediester in the presence of catalytic Yb(OTf)₃. The products are pyrrolidines in which the major diastereomer bears a cis relationship between substituents at the 2- and 5-positions. In most cases the diastereoselectivity is greater than 10:1.

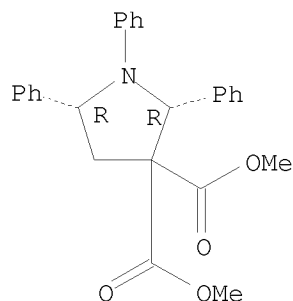
IT 866454-02-6P 866454-06-0P 866454-09-3P
866454-10-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of N-substituted pyrrolidines via Yb(OTf)₃ catalyzed
 diastereoselective cycloaddn. of primary amines/anilines, aldehydes,
 and 1,1-cyclopropanediester)

RN 866454-02-6 CAPLUS

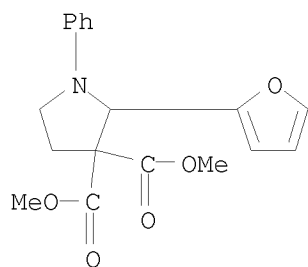
CN 3,3-Pyrrolidinedicarboxylic acid, 1,2,5-triphenyl-, 3,3-dimethyl ester,
 (2R,5R)-rel- (CA INDEX NAME)

Relative stereochemistry.



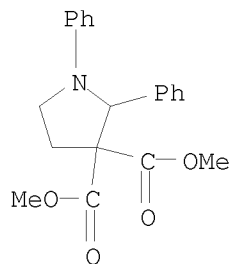
RN 866454-06-0 CAPLUS

CN 3,3-Pyrrolidinedicarboxylic acid, 2-(2-furanyl)-1-phenyl-, 3,3-dimethyl
 ester (CA INDEX NAME)



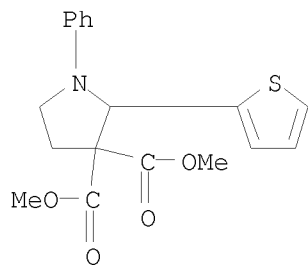
RN 866454-09-3 CAPLUS

CN 3,3-Pyrrolidinedicarboxylic acid, 1,2-diphenyl-, 3,3-dimethyl ester (CA
 INDEX NAME)



RN 866454-10-6 CAPLUS

CN 3,3-Pyrrolidinedicarboxylic acid, 1-phenyl-2-(2-thienyl)-, 3,3-dimethyl
 ester (CA INDEX NAME)



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 43 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:779160 CAPLUS

DOCUMENT NUMBER: 144:488188

TITLE: New Tandem Reactions of Metal Carbenoids.
Intermolecular Formation of Azomethine Ylide from
Methyl 2-Diazo-2-phenylacetate and Schiff Base:
Intramolecular 1,3-Dipolar Cycloaddition
AUTHOR(S): Khlebnikov, A. F.; Novikov, M. S.; Bespokoev, A. A.;
Kostikov, R. R.; Kopf, J.; Starikova, Z. A.; Antipin,
M. Yu.

CORPORATE SOURCE: St. Petersburg State University, St. Petersburg,
198504, Russia

SOURCE: Russian Journal of Organic Chemistry (2005), 41(6),
922-932

CODEN: RJOCEQ; ISSN: 1070-4280

PUBLISHER: Pleiades Publishing, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:488188

AB Rhodium acetate-catalyzed decomposition of Me 2-diazo-2-phenylacetate in the presence of substituted N-methylbenzylideneamines possessing an activated alkenyl fragment (dipolarophile) in the side chain gives products of intramol. cycloaddn. of intermediate Z,E- and E,Z-azomethine ylides. The cycloaddn. is regioselective, and the products are hexahydrochromeno[4,3-b]pyrrole derivs. The stereoselectivity of the process depends on the temperature. In the temperature range from 20 to 80°C, the major stereoisomer is that with cis junction of the tetrahydropyran and pyrrolidine rings. N-Phenylazomethine ylides generated from Me 2-diazo-2-phenylacetate and alkyl 4-[2-(phenyliminomethyl)phenoxy]-2-butenates at 40°C undergo cyclization to aziridines at a higher rate, as compared to the rate of cycloaddn. to the internal dipolarophile. N-Phenylazomethine ylides generated by thermolysis of the corresponding aziridine or by the "deprotonation" method react with equal regio- and stereoselectivity to give intramol. cycloaddn. products, hexahydrochromeno[4,3-b]pyrrole derivs. with trans-fused tetrahydropyran and pyrrolidine rings. Anal. of the exptl. and calcn. data suggests preference of the endo transition state in the cycloaddn. of the examined azomethine ylides.

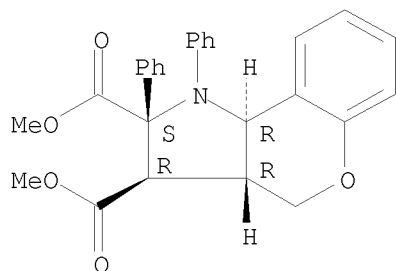
IT 887487-85-6P

RL: PRP (Properties); PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)
(crystallog.; regio- and stereoselective intramol. 1,3-dipolar cycloaddn. of azomethine ylide from Me 2-diazo-2-phenylacetate and Schiff base)

RN 887487-85-6 CAPLUS

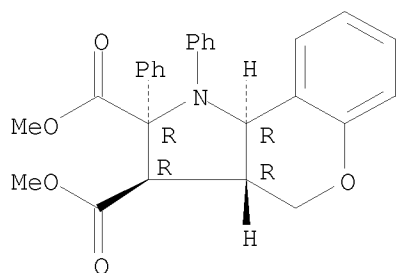
CN [1]Benzopyrano[4,3-b]pyrrole-2,3-dicarboxylic acid, 1,2,3,3a,4,9b-hexahydro-1,2-diphenyl-, 2,3-dimethyl ester, (2R,3S,3aS,9bS)-rel- (CA INDEX NAME)

Relative stereochemistry.



IT 887487-87-8P
RL: BYP (Byproduct); PUR (Purification or recovery); PREP (Preparation)
(regio- and stereoselective intramol. 1,3-dipolar cycloaddn. of
azomethine ylide from Me 2-diazo-2-phenylacetate and Schiff base)
RN 887487-87-8 CAPLUS
CN [1]Benzopyrano[4,3-b]pyrrole-2,3-dicarboxylic acid, 1,2,3,3a,4,9b-
hexahydro-1,2-diphenyl-, 2,3-dimethyl ester, (2R,3R,3aR,9bR)-rel- (CA
INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 44 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:618408 CAPLUS
DOCUMENT NUMBER: 143:386609
TITLE: Proximity effects: the observation by 1H NMR of steric
compression of the methano bridge protons of
polycyclic norbornanes possessing adjacent carbon,
oxygen and nitrogen bridges
AUTHOR(S): Margetic, Davor; Johnston, Martin R.; Warrenner, Ronald
N.; Butler, Douglas N.
CORPORATE SOURCE: Centre for Molecular Architecture, Central Queensland
University, Queensland, 4701, Australia
SOURCE: International Electronic Conferences on Synthetic
Organic Chemistry, 5th, 6th, Sept. 1-30, 2001 and 2002
[and] 7th, 8th, Nov. 1-30, 2003 and 2004 (2004),
1420-1428. Editor(s): Seijas, Julio A. Molecular
Diversity Preservation International: Basel, Switz.
CODEN: 69GTCO
DOCUMENT TYPE: Conference; (computer optical disk)
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:386609
AB Proximity effects of neighboring heteroatom bridges (oxygen, nitrogen)

cause steric compression shifts in the ¹H NMR chemical shifts of the bridge methano protons in fused norbornanes. This observation provides a simple 2-dimensional NMR method for elucidating the stereochem. outcome of cycloaddn. reactions that produce fused norbornane structures.

IT 866625-96-9

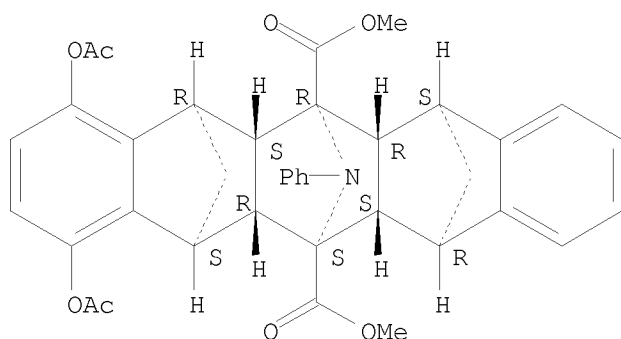
RL: PRP (Properties)

(proximity effects and ¹H NMR observations of steric compression of methano bridge protons of polycyclic norbornanes possessing adjacent carbon, oxygen and nitrogen bridges)

RN 866625-96-9 CAPLUS

CN 5,14:7,12-Dimethanopentacen-6,13-imine-6,13-dicarboxylic acid, 1,4-bis(acetyloxy)-5,5a,6a,7,12,12a,13a,14-octahydro-16-phenyl-, dimethyl ester, (5R,5aS,6R,6aR,7S,12R,12aS,13S,13aR,14S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 45 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:449667 CAPLUS

DOCUMENT NUMBER: 142:481953

TITLE: Preparation of pyridylpyrrolidinedicarboxamides, asymmetric acylation catalysts containing them, and preparation of optically active compounds using them

INVENTOR(S): Kawabata, Takeo

PATENT ASSIGNEE(S): Tokuyama Corp., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 19 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

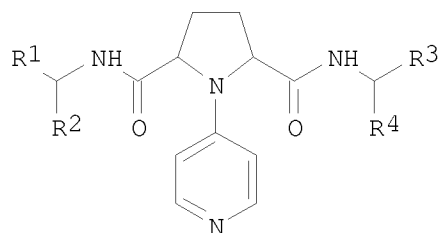
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

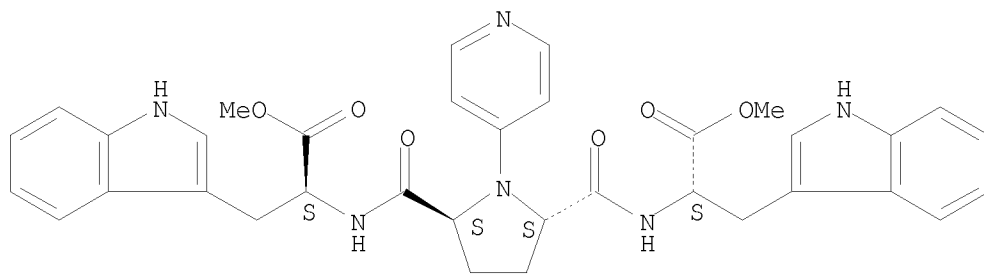
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2005132746	A	20050526	JP 2003-368239	20031029
PRIORITY APPLN. INFO.:			JP 2003-368239	20031029
OTHER SOURCE(S):	MARPAT	142:481953		

GI



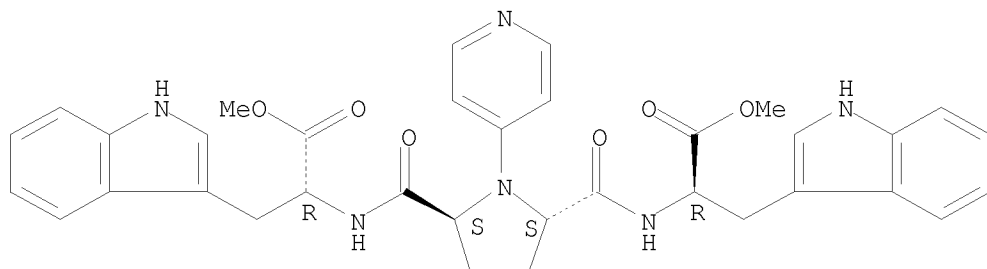
- AB The carboxamides I [R1, R3 = H, C1-6 alkoxycarbonyl; R2, R4 = H, C≤10 aromatic hydrocarbyl, (C≤10 aromatic heterocycle-substituted) C≤6 alkyl; R1 = R2 ≠ H; R3 = R4 ≠ H] are prepared by amidation of 1-(4-pyridyl)pyrrolidine-2,5-dicarboxylic acid with H2NCHR1R2 (R1, R2 = same as I) and H2NCHR3R4 (R3, R4 = same as I) using condensing agents. The catalysts comprise I with ≥50% optical purity. Meso-1,2-cyclohexanediol was acylated by isobutyric anhydride in the presence of (2S,5S)-1-(4-pyridyl)-2,5-bis[N-[(1S)-1-methoxycarbonyl-2-(3-indolyl)ethyl]carbamoyl]pyrrolidine and 2,4,6-collidine in CHCl3 at 20° for 4 h to give monoester with 73% ee and 85% selectivity.
- IT 852204-84-3P 852204-85-4P 852204-86-5P
852204-87-6P 852204-88-7P 852204-89-8P
852204-90-1P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation);
USES (Uses)
(preparation of optically active pyridylpyrrolidinedicarboxamides as asym. acylation catalysts)
- RN 852204-84-3 CAPLUS
- CN L-Tryptophan, N,N'-[[[(2S,5S)-1-(4-pyridinyl)-2,5-pyrrolidinediyl]dicarbonyl]bis-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



- RN 852204-85-4 CAPLUS
- CN D-Tryptophan, N,N'-[[[(2S,5S)-1-(4-pyridinyl)-2,5-pyrrolidinediyl]dicarbonyl]bis-, dimethyl ester (9CI) (CA INDEX NAME)

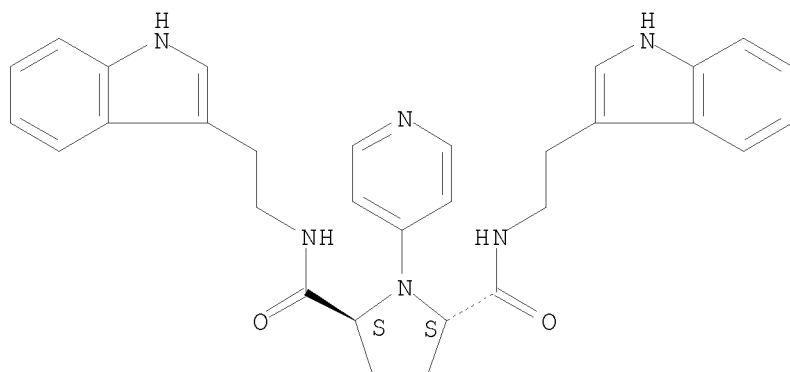
Absolute stereochemistry. Rotation (-).



RN 852204-86-5 CAPLUS

CN 2,5-Pyrrolidinedicarboxamide, N2,N5-bis[2-(1H-indol-3-yl)ethyl]-1-(4-pyridinyl)-, (2S,5S)- (CA INDEX NAME)

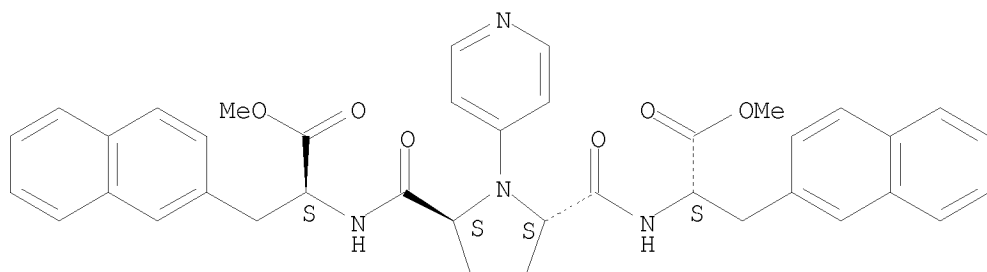
Absolute stereochemistry. Rotation (+).



RN 852204-87-6 CAPLUS

CN 2-Naphthalenepropanoic acid, α, α' -[[(2S,5S)-1-(4-pyridinyl)-2,5-pyrrolidinediyl]bis(carbonylimino)]bis-, dimethyl ester, (α S, α' S)- (9CI) (CA INDEX NAME)

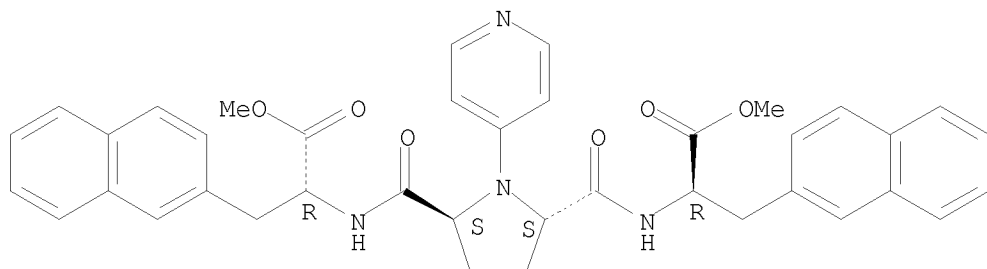
Absolute stereochemistry. Rotation (+).



RN 852204-88-7 CAPLUS

CN 2-Naphthalenepropanoic acid, α, α' -[[(2S,5S)-1-(4-pyridinyl)-2,5-pyrrolidinediyl]bis(carbonylimino)]bis-, dimethyl ester, (α R, α' R)- (9CI) (CA INDEX NAME)

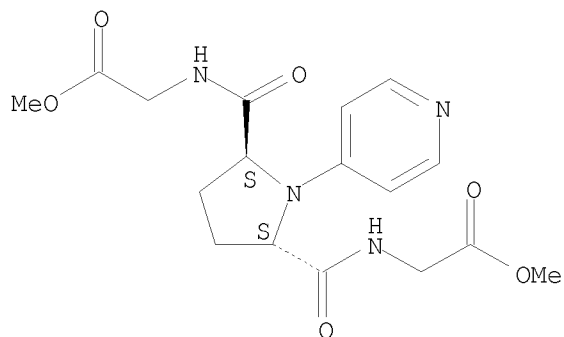
Absolute stereochemistry. Rotation (-).



RN 852204-89-8 CAPLUS

CN Glycine, N,N'-[[1-(4-pyridinyl)-2,5-pyrrolidinediyl]dicarbonyl]bis-, dimethyl ester (9CI) (CA INDEX NAME)

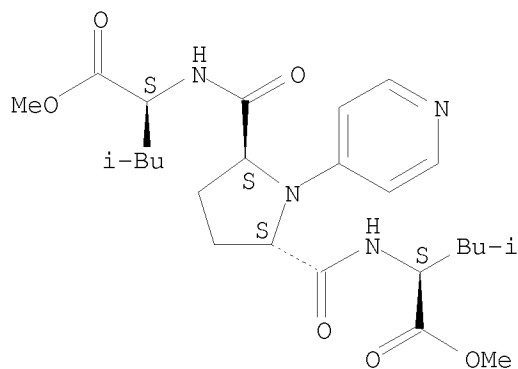
Absolute stereochemistry. Rotation (-).



RN 852204-90-1 CAPLUS

CN L-Leucine, N,N'-[[1-(4-pyridinyl)-2,5-pyrrolidinediyl]dicarbonyl]bis-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



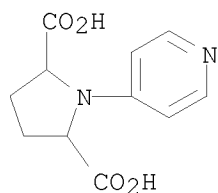
IT 852204-92-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of optically active pyridylpyrrolidinedicarboxamides as asym. acylation catalysts)

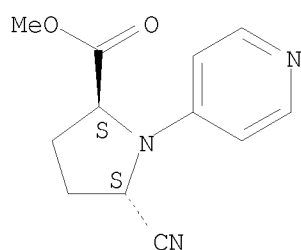
RN 852204-92-3 CAPLUS

CN 2,5-Pyrrolidinedicarboxylic acid, 1-(4-pyridinyl)- (CA INDEX NAME)



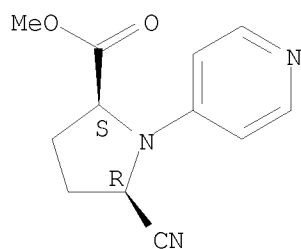
IT 852204-80-9P 852204-81-0P 852204-82-1P
 852204-83-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation of optically active pyridylpyrrolidinedicarboxamides as asym.
 acylation catalysts)
 RN 852204-80-9 CAPLUS
 CN L-Proline, 5-cyano-1-(4-pyridinyl)-, methyl ester, (5S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



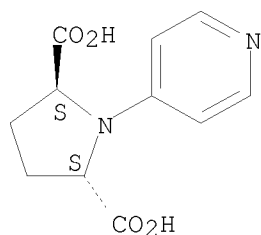
RN 852204-81-0 CAPLUS
 CN L-Proline, 5-cyano-1-(4-pyridinyl)-, methyl ester, (5R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 852204-82-1 CAPLUS
 CN 2,5-Pyrrolidinedicarboxylic acid, 1-(4-pyridinyl)-, hydrochloride (1:1),
 (2S,5S)- (CA INDEX NAME)

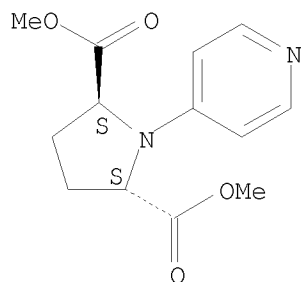
Absolute stereochemistry. Rotation (-).



● HCl

RN 852204-83-2 CAPLUS
 CN 2,5-Pyrrolidinedicarboxylic acid, 1-(4-pyridinyl)-, 2,5-dimethyl ester,
 (2S,5S)- (CA INDEX NAME)

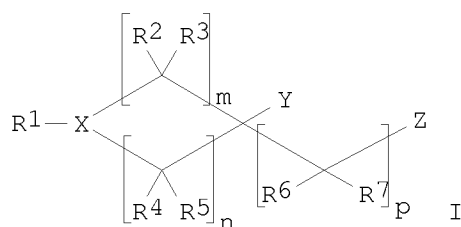
Absolute stereochemistry.



L3 ANSWER 46 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2005:369273 CAPLUS
 DOCUMENT NUMBER: 142:430299
 TITLE: Preparation of novel piperidine and
 cyclohexanecarbonitrile derivatives effective in
 enhancing LDL receptor manifestation
 INVENTOR(S): Ban, Hitoshi; Ohnuma, Satoshi; Tsuboya, Norie; Asano,
 Shigehiro
 PATENT ASSIGNEE(S): Sumitomo Pharmaceuticals Co., Ltd., Japan
 SOURCE: PCT Int. Appl., 209 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005037269	A1	20050428	WO 2004-JP15773	20041019
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,			

SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
 SN, TD, TG
 EP 1679069 A1 20060712 EP 2004-792910 20041019
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK
 US 20070078120 A1 20070405 US 2006-576581 20060420
 PRIORITY APPLN. INFO.: JP 2003-361256 A 20031021
 WO 2004-JP15773 W 20041019
 OTHER SOURCE(S): MARPAT 142:430299
 GI



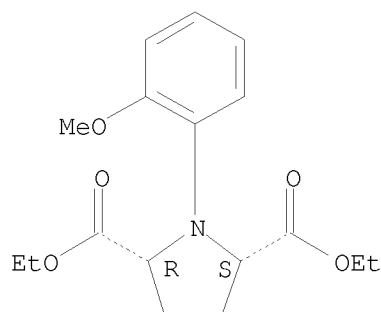
AB Drugs for enhancing LDL receptor manifestation contains compds. represented by the following formula (I), prodrugs thereof, or pharmaceutically acceptable salts of either [m, n, p = 0-4, provided that 3≤m+n≤8; X = N, each (un)substituted CH; Y = each (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, or aromatic group, COY; R1 = H, each (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, 3- to 8-membered saturated heterocyclyl containing one (un)substituted NH or O, aromatic group, COR14; R14 = each (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, or aromatic group; R2-R7 = H, OH, each (un)substituted alkyl, alkoxy, alkoxycarbonyl, aralkyl, heteroarylalkyl, aralkyloxy, or heteroarylalkyloxy; or one or a plural combination of R2 and R3, R4 and R5, or R6 and R7 = oxo; or R2 and R4 together = alkylene; two of R2-R5 are on the adjacent carbon atom to form a double bond; Z = H, OH, CO2H, cyano, phthalimido, halo, each (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, or aromatic group, etc.] as active ingredients. These compds. are effective in enhancing low d. lipoprotein (LDL) receptor manifestation and lowering blood concentration of LDL cholesterol and are useful as therapeutic agents for treating hyperlipemia and arteriosclerosis. Thus, 0.019 mL benzyl bromide was added to a suspension of 40 mg 4-(3-methoxyphenyl)-1,4'-bipiperidine-4-carbonitrile dihydrochloride and 92.6 mg K2CO3 in 1.0 mL DMF under ice-cooling, and the resulting mixture was warmed to room temperature, stirred overnight, and quenched by adding water to give, after workup and silica gel chromatog., 15.6 mg 1'-benzyl-4-(3-methoxyphenyl)-1,1'-bipiperidine-4-carbonitrile (II). II at 10 μM and N-benzyl-4-(3-methoxyphenyl)-1-(pyrimidin-2-yl)piperidine-4-carbothioamide at 3 μM enhanced the LDL receptor activity by 135 and 195%, resp.

IT 850887-29-5P, Diethyl cis-1-(2-methoxyphenyl)pyrrolidine-2,5-dicarboxylate
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of novel piperidine and cyclohexanecarbonitrile derivs. as enhancers for LDL receptor manifestation, hypolipidemics, and antiarteriosclerotics)

RN 850887-29-5 CAPLUS

CN 2,5-Pyrrolidinedicarboxylic acid, 1-(2-methoxyphenyl)-, 2,5-diethyl ester, (2S,5R)-rel- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 47 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:238948 CAPLUS

DOCUMENT NUMBER: 142:317078

TITLE: Preparation of pyrrolidine-2-carbonitrile derivatives and their use as inhibitors of dipeptidyl peptidase-IV (DPP-IV)

INVENTOR(S): Pei, Zhonghua; Li, Xiaofeng; Longenecker, Kenton L.; Sham, Hing L.; Wiedeman, Paul E.

PATENT ASSIGNEE(S): Abbott Laboratories, USA

SOURCE: PCT Int. Appl., 182 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005023762	A1	20050317	WO 2004-US28886	20040907
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			

PRIORITY APPLN. INFO.: US 2003-655428 A 20030904

OTHER SOURCE(S): CASREACT 142:317078; MARPAT 142:317078

AB The invention relates to 1-(5-ROCH₂-substituted prolyl)pyrrolidine-2-carbonitriles (R is substituted Ph, 2-, 3-, or 4-pyridyl, or 4-quinolyl) or their pharmaceutically-acceptable salts or prodrugs, which inhibit dipeptidyl peptidase IV (DPP-IV) and are useful for the prevention or treatment of diabetes, especially type II diabetes, as well as hyperglycemia, syndrome X, hyperinsulinemia, β -cell failure, obesity, satiety disorders, atherosclerosis, and various immunomodulatory diseases. Thus, (2S)-1-[(5R)-5-[(4-carboxynaphthalen-1-yloxy)methyl]-L-prolyl]pyrrolidine-2-carbonitrile, prepared via N-acylation and etherification reactions, was

evaluated for ability to treat diabetes using an acute oral glucose tolerance test (8 AUGC = 7,600 mg/mL/dL at 1.0 mg/kg vs. 9,900 mg/mL/dL for the control).

IT 847942-13-6P

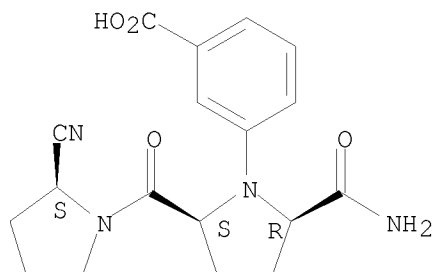
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyrrolidinecarbonitrile derivs. as inhibitors of dipeptidyl peptidase-IV)

RN 847942-13-6 CAPLUS

CN Benzoic acid, 3-[(2R,5S)-2-(aminocarbonyl)-5-[[[(2S)-2-cyano-1-pyrrolidinyl]carbonyl]-1-pyrrolidinyl]- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 48 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:86460 CAPLUS

DOCUMENT NUMBER: 142:328905

TITLE: Structure-based design of potent and selective inhibitors of collagenase-3 (MMP-13)

AUTHOR(S): Kim, Soong-Hoon; Pudzianowski, Andrew T.; Leavitt, Kenneth J.; Barbosa, Joseph; McDonnell, Patricia A.; Metzler, William J.; Rankin, Bruce M.; Liu, Richard; Vaccaro, Wayne; Pitts, William

CORPORATE SOURCE: Bristol Myers Squibb Co., Pharmaceutical Research Institute, Princeton, NJ, 08560, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(4), 1101-1106

CODEN: BMCLE8; ISSN: 0960-894X

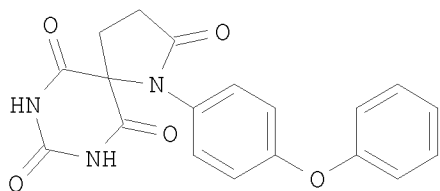
PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:328905

GI



I

AB Computer aided drug design led to a new class of spiro-barbiturates (e.g., I, MMP-13 $K_i = 4.7$ nM) that are potent inhibitors of MMP-13.

IT 848773-40-0P 848773-41-1P 848773-42-2P

848773-48-8P 848773-49-9P 848773-50-2P

848773-51-3P 848773-52-4P 848773-53-5P

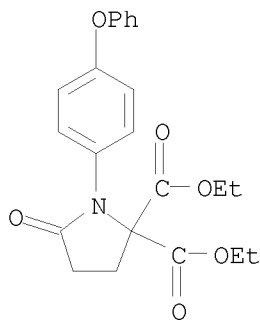
848773-54-6P 848773-55-7P 848773-56-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(Structure-based design of potent and selective inhibitors of collagenase-3)

RN 848773-40-0 CAPLUS

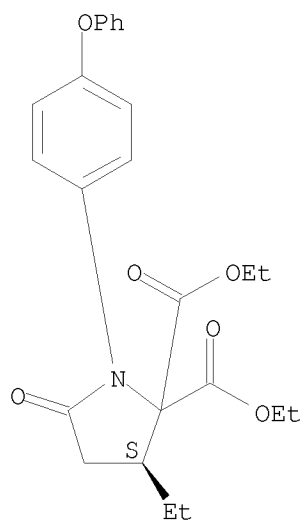
CN 2,2-Pyrrolidinedicarboxylic acid, 5-oxo-1-(4-phenoxyphenyl)-, 2,2-diethyl ester (CA INDEX NAME)



RN 848773-41-1 CAPLUS

CN 2,2-Pyrrolidinedicarboxylic acid, 3-ethyl-5-oxo-1-(4-phenoxyphenyl)-, 2,2-diethyl ester, (3S)- (CA INDEX NAME)

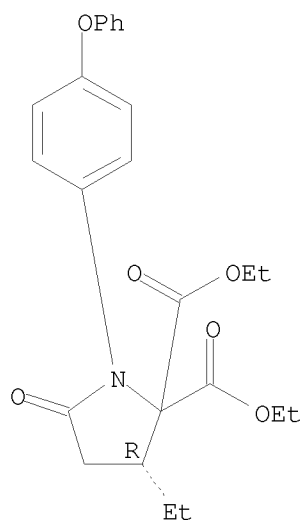
Absolute stereochemistry.



RN 848773-42-2 CAPLUS

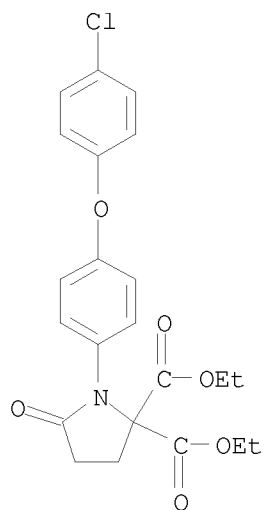
CN 2,2-Pyrrolidinedicarboxylic acid, 3-ethyl-5-oxo-1-(4-phenoxyphenyl)-,
2,2-diethyl ester, (3R)- (CA INDEX NAME)

Absolute stereochemistry.



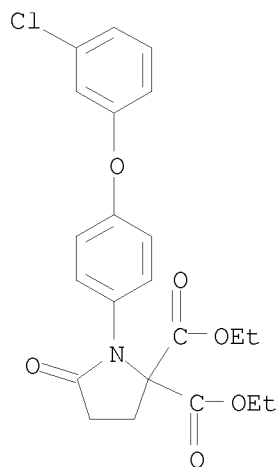
RN 848773-48-8 CAPLUS

CN 2,2-Pyrrolidinedicarboxylic acid, 1-[4-(4-chlorophenoxy)phenyl]-5-oxo-,
2,2-diethyl ester (CA INDEX NAME)



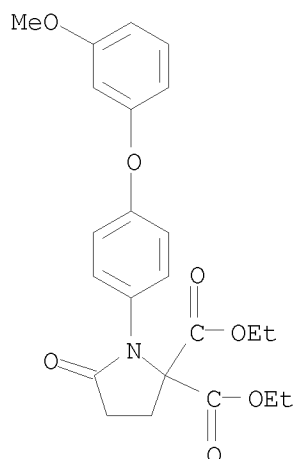
RN 848773-49-9 CAPLUS

CN 2,2-Pyrrolidinedicarboxylic acid, 1-[4-(3-chlorophenoxy)phenyl]-5-oxo-,
2,2-diethyl ester (CA INDEX NAME)



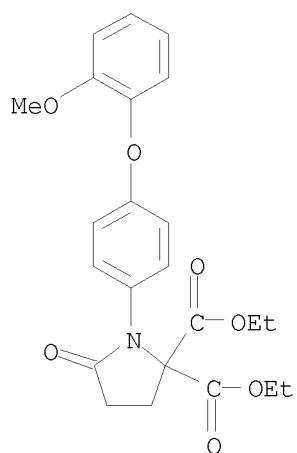
RN 848773-50-2 CAPLUS

CN 2,2-Pyrrolidinedicarboxylic acid, 1-[4-(3-methoxyphenoxy)phenyl]-5-oxo-,
2,2-diethyl ester (CA INDEX NAME)



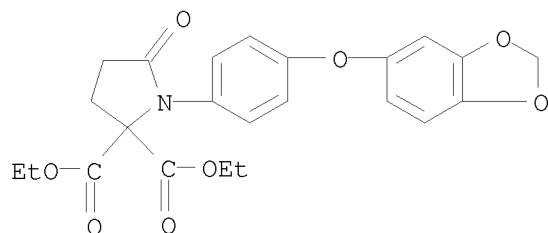
RN 848773-51-3 CAPLUS

CN 2,2-Pyrrolidinedicarboxylic acid, 1-[4-(2-methoxyphenoxy)phenyl]-5-oxo-,
2,2-diethyl ester (CA INDEX NAME)



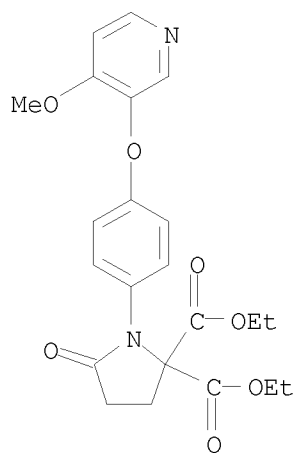
RN 848773-52-4 CAPLUS

CN 2,2-Pyrrolidinedicarboxylic acid, 1-[4-(1,3-benzodioxol-5-yloxy)phenyl]-5-oxo-,
2,2-diethyl ester (CA INDEX NAME)



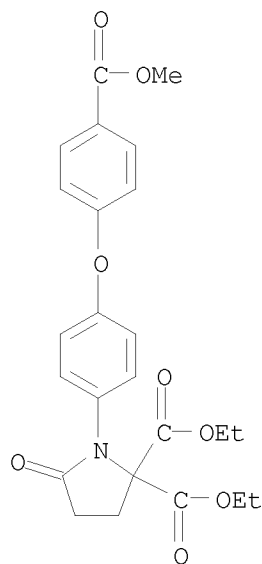
RN 848773-53-5 CAPLUS

CN 2,2-Pyrrolidinedicarboxylic acid, 1-[4-[(4-methoxy-3-pyridinyl)oxy]phenyl]-5-oxo-,
2,2-diethyl ester (CA INDEX NAME)



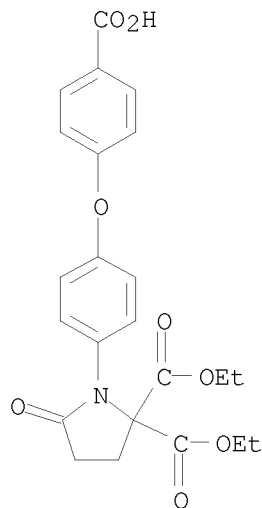
RN 848773-54-6 CAPLUS

CN 2,2-Pyrrolidinedicarboxylic acid, 1-[4-[4-(methoxycarbonyl)phenoxy]phenyl]-5-oxo-, 2,2-diethyl ester (CA INDEX NAME)

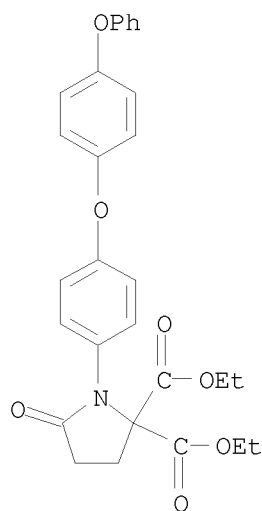


RN 848773-55-7 CAPLUS

CN 2,2-Pyrrolidinedicarboxylic acid, 1-[4-(4-carboxyphenoxy)phenyl]-5-oxo-, 2,2-diethyl ester (CA INDEX NAME)



RN 848773-56-8 CAPLUS
 CN 2,2-Pyrrolidinedicarboxylic acid, 5-oxo-1-[4-(4-phenoxyphenoxy)phenyl]-,
 2,2-diethyl ester (CA INDEX NAME)



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 49 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2005:85523 CAPLUS
 DOCUMENT NUMBER: 142:336502
 TITLE: Diastereoselective Synthesis of Pyrrolidines Using a
 Nitron/Cyclopropane Cycloaddition: Synthesis of the
 Tetracyclic Core of Nakadomarin A
 AUTHOR(S): Young, Ian S.; Williams, Justin L.; Kerr, Michael A.
 CORPORATE SOURCE: Department of Chemistry, The University of Western
 Ontario, London, ON, N6A 5B7, Can.
 SOURCE: Organic Letters (2005), 7(5), 953-955
 CODEN: ORLEF7; ISSN: 1523-7060
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal

LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:336502
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The synthesis of the tetracyclic core, I, of nakadomarin A is described. The core contains all the heterocycles and the required stereocenters found in the natural product and provides a promising route to the target itself. The strategy utilizes a general, diastereoselective pyrrolidine synthesis that proceeds via a homo 3 + 2 dipolar cycloaddn. For example, the intermediate amino alc. II was generated by cleavage of the N-O bond of the oxazine III and recyclization of II gave a tricyclic pyrrolidine which was subsequently transformed into I. The scope of this methodol. is also described.

IT 848586-89-0P 848586-91-4P

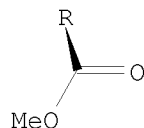
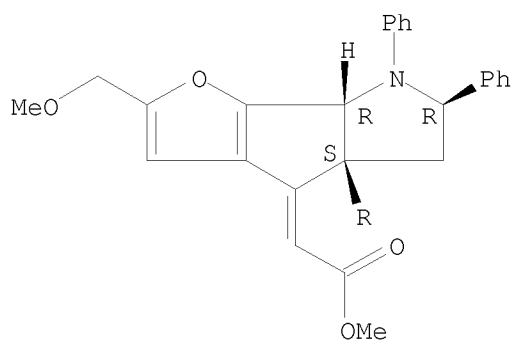
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(diastereoselective synthesis of pyrrolidines via nitron/cyclopropane cycloaddn. and application to synthesis of tetracyclic core of nakadomarin A)

RN 848586-89-0 CAPLUS

CN Furo[3',2':4,5]cyclopenta[1,2-b]pyrrole-4a(4H)-carboxylic acid, 5,6,7,7a-tetrahydro-2-(methoxymethyl)-4-(2-methoxy-2-oxoethylidene)-6,7-diphenyl-, methyl ester, (4aR,6S,7aS)-rel- (CA INDEX NAME)

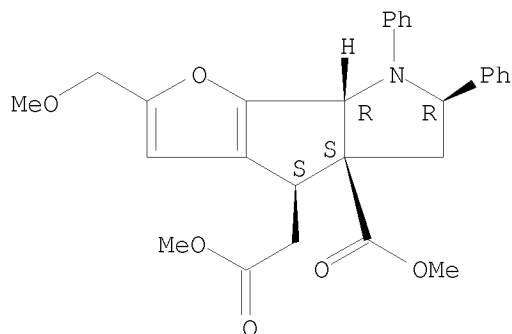
Relative stereochemistry.
Double bond geometry unknown.



RN 848586-91-4 CAPLUS

CN Furo[3',2':4,5]cyclopenta[1,2-b]pyrrole-4(4H)-acetic acid, 5,6,7,7a-tetrahydro-4a-(methoxycarbonyl)-2-(methoxymethyl)-6,7-diphenyl-, methyl ester, (4R,4aR,6S,7aS)-rel- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 50 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:76721 CAPLUS

DOCUMENT NUMBER: 142:430075

TITLE: Synthesis of ethyl cis- and trans-4-chloro-5-oxo-1,2-diphenyl-pyrrolidine-2-carboxylate

AUTHOR(S): Martirosyan, A. O.; Hovhanesyan, V. E.; Gasparyan, S. P.; Karapetyan, A. A.; Panosyan, G. A.; Martirosyan, V. O.

CORPORATE SOURCE: A. L. Mndzhoyan Institute of Fine Chemistry, Armenian Republic National Academy of Sciences, Yerevan, 375014, Armenia

SOURCE: Chemistry of Heterocyclic Compounds (New York, NY, United States) (2004), 40(8), 1007-1008
CODEN: CHCCAL; ISSN: 0009-3122

PUBLISHER: Springer Science+Business Media, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:430075

AB Et cis- and trans-4-chloro-5-oxo-1,2-diphenylpyrrolidine-2-carboxylate were synthesized by the cyclization of Et N-(α,β -dichloropropionyl)-N-phenyl- α -aminophenylacetate.

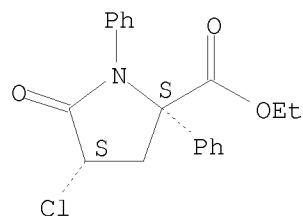
IT 850836-21-4P 850836-22-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of Et cis- and trans-4-chloro-5-oxo-1,2-diphenyl-pyrrolidine-2-carboxylate by cyclization of Et N-(α,β -dichloropropionyl)-N-phenyl- α -aminophenylacetate)

RN 850836-21-4 CAPLUS

CN D-Proline, 4-chloro-5-oxo-1,2-diphenyl-, ethyl ester, (4S)-rel- (CA INDEX NAME)

Relative stereochemistry.

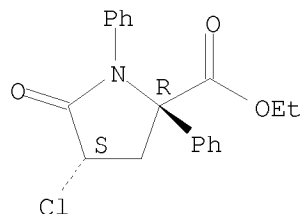


RN 850836-22-5 CAPLUS

CN D-Proline, 4-chloro-5-oxo-1,2-diphenyl-, ethyl ester, (4R)-rel- (9CI) (CA

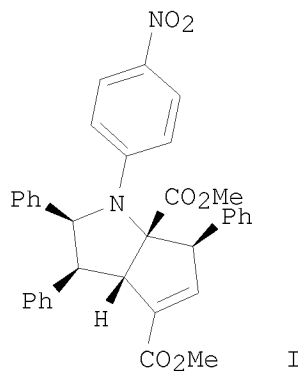
INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 51 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:8762 CAPLUS
DOCUMENT NUMBER: 142:219110
TITLE: Stereoselective synthesis of bicyclic pyrrolidines by a rhodium-catalyzed cascade process
AUTHOR(S): Yan, Ming; Jacobsen, Neil; Hu, Wenhao; Gronenberg, Luisa S.; Doyle, Michael P.; Colyer, John T.; Bykowski, Darren
CORPORATE SOURCE: Department of Chemistry, University of Maryland, College Park, MD, 20742, USA
SOURCE: Angewandte Chemie, International Edition (2004), 43(48), 6713-6716
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:219110
GI



AB Multiple C-C bonds were formed in an unprecedented reaction of an ylide with an excess of a rhodium-stabilized carbene. The cascade cyclization of the intermediates, formed from the three components, gave bicyclic pyrrolidines, e.g., I, with excellent diastereoselectivity.

IT 844437-12-3P

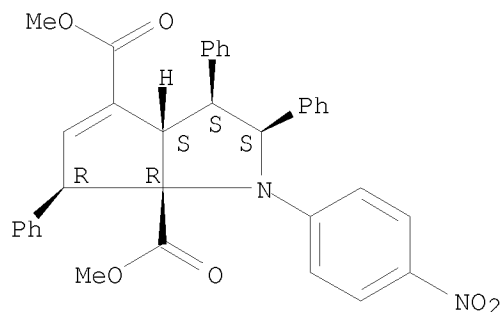
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (stereoselective preparation and crystal structure of N-(nitrophenyl)triphenylazabicyclooctenedicarboxylate via rhodium-catalyzed stereoselective cyclization of N-

(benzylidene)nitroaniline with diazo(phenyl)butenoate)

RN 844437-12-3 CAPLUS

CN Cyclopenta[b]pyrrole-4,6a(1H)-dicarboxylic acid, 2,3,3a,6-tetrahydro-1-(4-nitrophenyl)-2,3,6-triphenyl-, 4,6a-dimethyl ester, (2S,3S,3aS,6R,6aR)- (CA INDEX NAME)

Absolute stereochemistry.



IT 844437-13-4P 844437-14-5P 844437-15-6P

844437-16-7P 844437-17-8P 844437-18-9P

844437-19-0P 844437-20-3P 844437-21-4P

844437-22-5P 844437-23-6P 844437-24-7P

844437-25-8P

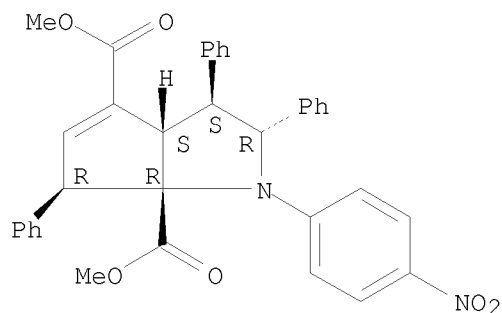
RL: SPN (Synthetic preparation); PREP (Preparation)

(stereoselective preparation of tetra(aryl)azabicyclooctenedicarboxylates via rhodium-catalyzed stereoselective cyclization of N-(benzylidene)anilines with diazo(phenyl)butenoate)

RN 844437-13-4 CAPLUS

CN Cyclopenta[b]pyrrole-4,6a(1H)-dicarboxylic acid, 2,3,3a,6-tetrahydro-1-(4-nitrophenyl)-2,3,6-triphenyl-, 4,6a-dimethyl ester, (2R,3S,3aS,6R,6aR)- (CA INDEX NAME)

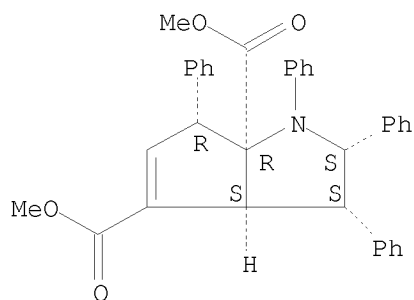
Absolute stereochemistry.



RN 844437-14-5 CAPLUS

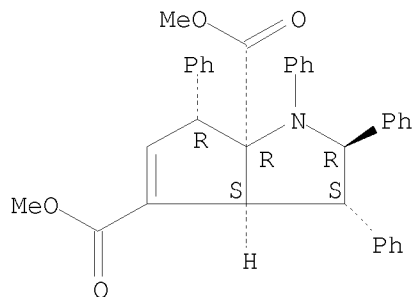
CN Cyclopenta[b]pyrrole-4,6a(1H)-dicarboxylic acid, 2,3,3a,6-tetrahydro-1,2,3,6-tetraphenyl-, 4,6a-dimethyl ester, (2S,3S,3aS,6R,6aR)- (CA INDEX NAME)

Absolute stereochemistry.



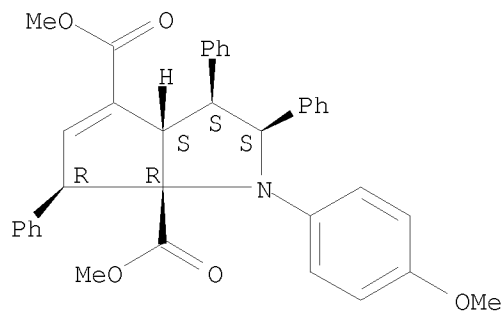
RN 844437-15-6 CAPLUS
 CN Cyclopenta[b]pyrrole-4,6a(1H)-dicarboxylic acid, 2,3,3a,6-tetrahydro-1,2,3,6-tetraphenyl-, 4,6a-dimethyl ester, (2R,3S,3aS,6R,6aR)- (CA INDEX NAME)

Absolute stereochemistry.



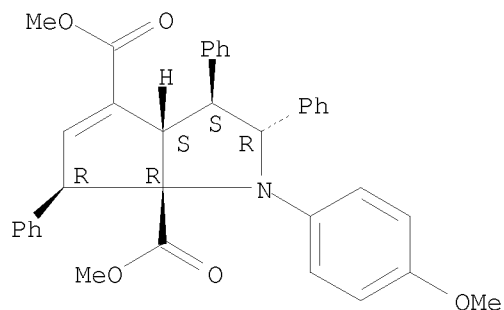
RN 844437-16-7 CAPLUS
 CN Cyclopenta[b]pyrrole-4,6a(1H)-dicarboxylic acid, 2,3,3a,6-tetrahydro-1-(4-methoxyphenyl)-2,3,6-triphenyl-, 4,6a-dimethyl ester, (2S,3S,3aS,6R,6aR)- (CA INDEX NAME)

Absolute stereochemistry.



RN 844437-17-8 CAPLUS
 CN Cyclopenta[b]pyrrole-4,6a(1H)-dicarboxylic acid, 2,3,3a,6-tetrahydro-1-(4-methoxyphenyl)-2,3,6-triphenyl-, 4,6a-dimethyl ester, (2R,3S,3aS,6R,6aR)- (CA INDEX NAME)

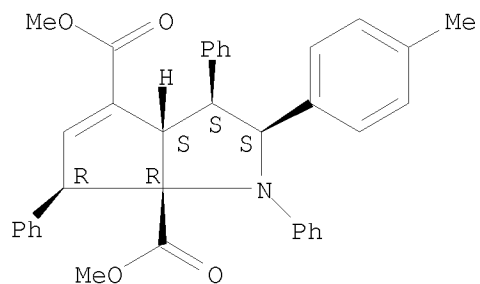
Absolute stereochemistry.



RN 844437-18-9 CAPLUS

CN Cyclopenta[b]pyrrole-4,6a(1H)-dicarboxylic acid, 2,3,3a,6-tetrahydro-2-(4-methylphenyl)-1,3,6-triphenyl-, 4,6a-dimethyl ester, (2S,3S,3aS,6R,6aR)- (CA INDEX NAME)

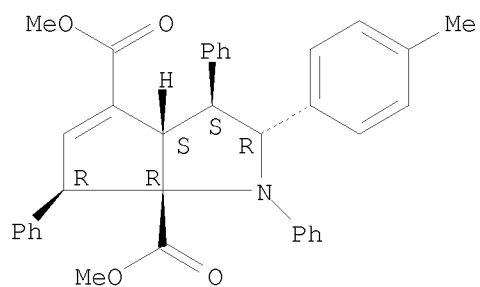
Absolute stereochemistry.



RN 844437-19-0 CAPLUS

CN Cyclopenta[b]pyrrole-4,6a(1H)-dicarboxylic acid, 2,3,3a,6-tetrahydro-2-(4-methylphenyl)-1,3,6-triphenyl-, 4,6a-dimethyl ester, (2R,3S,3aS,6R,6aR)- (CA INDEX NAME)

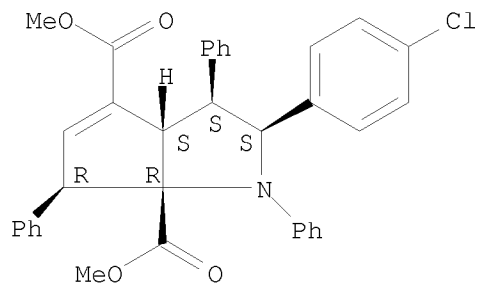
Absolute stereochemistry.



RN 844437-20-3 CAPLUS

CN Cyclopenta[b]pyrrole-4,6a(1H)-dicarboxylic acid, 2-(4-chlorophenyl)-2,3,3a,6-tetrahydro-1,3,6-triphenyl-, 4,6a-dimethyl ester, (2S,3S,3aS,6R,6aR)- (CA INDEX NAME)

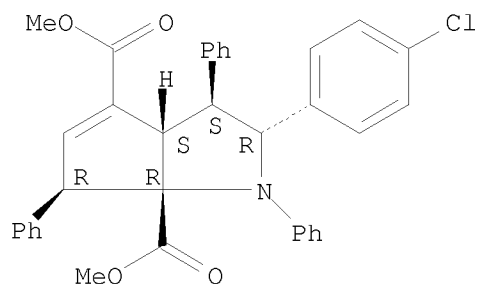
Absolute stereochemistry.



RN 844437-21-4 CAPLUS

CN Cyclopenta[b]pyrrole-4,6a(1H)-dicarboxylic acid, 2-(4-chlorophenyl)-2,3,3a,6-tetrahydro-1,3,6-triphenyl-, 4,6a-dimethyl ester, (2R,3S,3aS,6R,6aR)- (CA INDEX NAME)

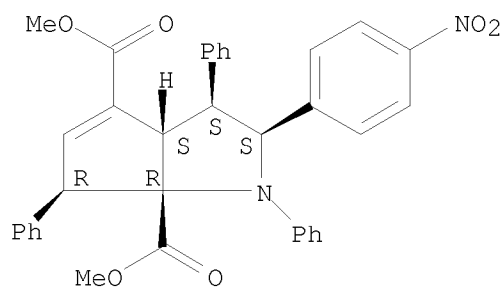
Absolute stereochemistry.



RN 844437-22-5 CAPLUS

CN Cyclopenta[b]pyrrole-4,6a(1H)-dicarboxylic acid, 2,3,3a,6-tetrahydro-2-(4-nitrophenyl)-1,3,6-triphenyl-, 4,6a-dimethyl ester, (2S,3S,3aS,6R,6aR)- (CA INDEX NAME)

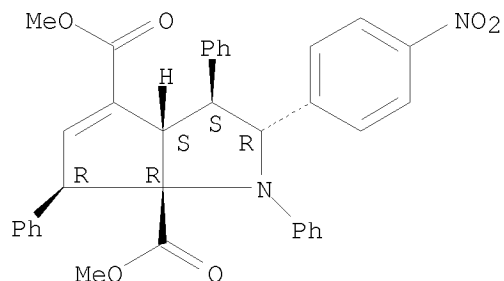
Absolute stereochemistry.



RN 844437-23-6 CAPLUS

CN Cyclopenta[b]pyrrole-4,6a(1H)-dicarboxylic acid, 2-(4-nitrophenyl)-1,3,6-triphenyl-, 4,6a-dimethyl ester, (2R,3S,3aS,6R,6aR)- (CA INDEX NAME)

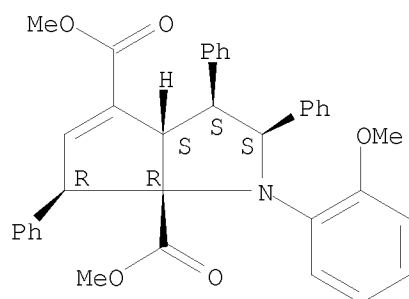
Absolute stereochemistry.



RN 844437-24-7 CAPLUS

CN Cyclopenta[b]pyrrole-4,6a(1H)-dicarboxylic acid, 2,3,3a,6-tetrahydro-1-(2-methoxyphenyl)-2,3,6-triphenyl-, 4,6a-dimethyl ester, (2S,3S,3aS,6R,6aR)-(CA INDEX NAME)

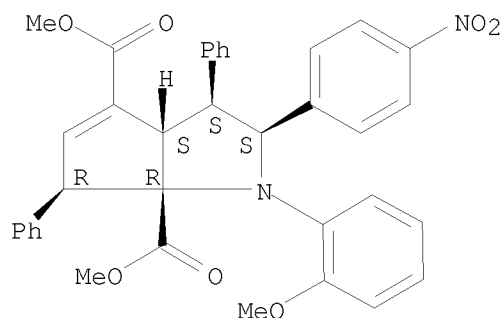
Absolute stereochemistry.



RN 844437-25-8 CAPLUS

CN Cyclopenta[b]pyrrole-4,6a(1H)-dicarboxylic acid, 2,3,3a,6-tetrahydro-1-(2-methoxyphenyl)-2-(4-nitrophenyl)-3,6-diphenyl-, 4,6a-dimethyl ester, (2S,3S,3aS,6R,6aR)-(CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

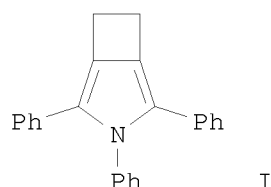
L3 ANSWER 52 OF 73 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:1066156 CAPLUS

DOCUMENT NUMBER: 142:155758

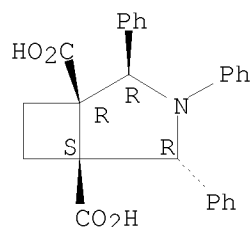
TITLE: 2,3,4-Triphenyl-3-azabicyclo[3.2.0]hepta-1,4-diene - facile ring-opening by electrophiles and novel reactions with dimethyl acetylenedicarboxylate

AUTHOR(S): Matsumoto, Kiyoshi; Goto, Sadahito; Hayashi, Naoto;
 Iida, Hirokazu; Uchida, Takane; Kakehi, Akikazu
 CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, Chiba Institute of
 Science, Chiba, 288-0025, Japan
 SOURCE: European Journal of Organic Chemistry (2004), (22),
 4667-4671
 CODEN: EJOCFK; ISSN: 1434-193X
 PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 142:155758
 GI



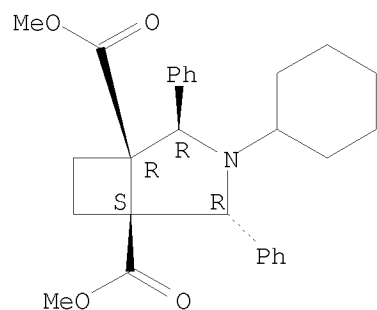
AB A 3-azabicyclo[3.2.0]hepta-1,4-diene I with no substituent in the
 cyclobutene moiety has been prepared I underwent extremely facile
 electrophilic attack at the β -position to give the ring-opened
 products, probably by a retro-Friedel-Crafts process. I reacted with
 di-Me acetylenedicarboxylate to afford the corresponding azepine.
 IT 828917-31-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation of azabicycloheptanedicarboxylic acids via hydrolysis of
 azabicycloheptanedicarboxylates)
 RN 828917-31-3 CAPLUS
 CN 3-Azabicyclo[3.2.0]heptane-1,5-dicarboxylic acid, 2,3,4-triphenyl-,
 (1R,2R,4R,5S)-rel- (CA INDEX NAME)

Relative stereochemistry.



IT 828917-30-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (stereoselective preparation of azabicycloheptanedicarboxylates via
 stereoselective dipolar cycloaddn. of aziridines to
 cyclobutenedicarboxylate)
 RN 828917-30-2 CAPLUS
 CN 3-Azabicyclo[3.2.0]heptane-1,5-dicarboxylic acid, 3-cyclohexyl-2,4-
 diphenyl-, 1,5-dimethyl ester, (1S,2S,4S,5R)-rel- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT:

35

THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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